

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA160RXA

PASSWORD:

LOGINID/PASSWORD REJECTED

The loginid and/or password sent to STN were invalid.
You either typed them incorrectly, or line noise may
have corrupted them.

Do you wish to retry the logon?

Enter choice (y/N):

Do you wish to use the same loginid and password?

Enter choice (y/N):

Enter new loginid (or press [Enter] for SSSPTA160RXA):

Enter new password:

LOGINID:

LOGINID:SSSPTA1600RXA

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	FEB 25	CA/CAPLUS - Russian Agency for Patents and Trademarks (ROSPATENT) added to list of core patent offices covered
NEWS	4	FEB 28	PATDPAFULL - New display fields provide for legal status data from INPADOC
NEWS	5	FEB 28	BABS - Current-awareness alerts (SDIs) available
NEWS	6	FEB 28	MEDLINE/LMEDLINE reloaded
NEWS	7	MAR 02	GBFULL: New full-text patent database on STN
NEWS	8	MAR 03	REGISTRY/ZREGISTRY - Sequence annotations enhanced
NEWS	9	MAR 03	MEDLINE file segment of TOXCENTER reloaded
NEWS	10	MAR 22	KOREAPAT now updated monthly; patent information enhanced
NEWS	11	MAR 22	Original IDE display format returns to REGISTRY/ZREGISTRY
NEWS	12	MAR 22	PATDPASPC - New patent database available
NEWS	13	MAR 22	REGISTRY/ZREGISTRY enhanced with experimental property tags

NEWS EXPRESS JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 15:22:16 ON 01 APR 2005

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 15:22:23 ON 01 APR 2005

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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 31 MAR 2005 HIGHEST RN 847735-80-2

DICTIONARY FILE UPDATES: 31 MAR 2005 HIGHEST RN 847735-80-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

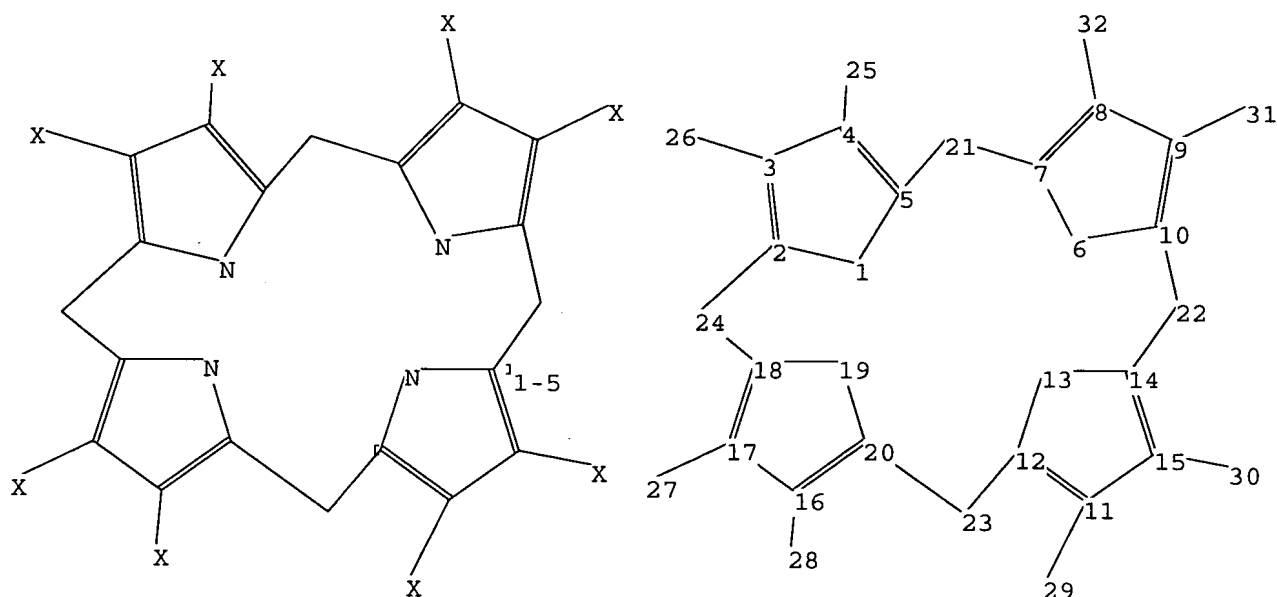
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Program Files\Stnexp\Queries\09939514.str



```

chain nodes :
25 26 27 28 29 30 31 32
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24
chain bonds :
3-26 4-25 8-32 9-31 11-29 15-30 16-28 17-27
ring bonds :
1-2 1-5 2-3 2-24 3-4 4-5 5-21 6-7 6-10 7-8 7-21 8-9 9-10 10-22 11-12
11-15 12-13 12-23 13-14 14-15 14-22 16-17 16-20 17-18 18-19 18-24 19-20
20-23
exact/norm bonds :
1-2 1-5 2-3 2-24 3-4 4-5 5-21 6-7 6-10 7-8 7-21 8-9 9-10 10-22 11-12
11-15 12-13 12-23 13-14 14-15 14-22 16-17 16-20 17-18 18-19 18-24 19-20
20-23
exact bonds :
3-26 4-25 8-32 9-31 11-29 15-30 16-28 17-27
isolated ring systems :
containing 1 :

```

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Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:CLASS 26:CLASS 27:CLASS 28:CLASS
29:CLASS 30:CLASS 31:CLASS 32:CLASS

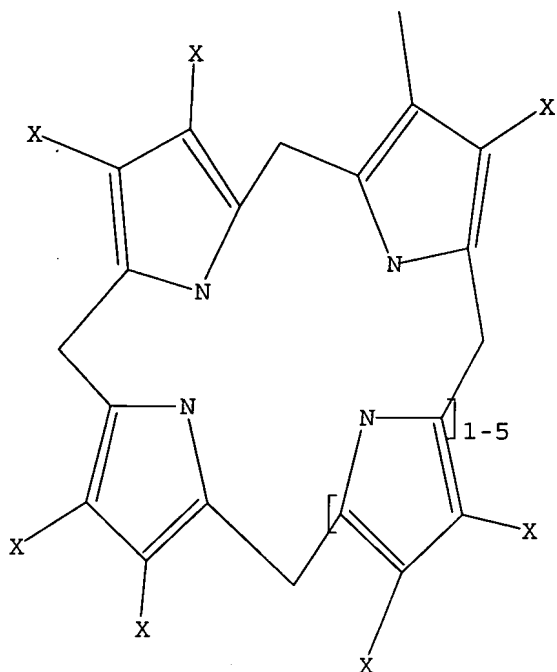
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L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 15:22:39 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 187 TO ITERATE

100.0% PROCESSED 187 ITERATIONS
SEARCH TIME: 00.00.01

11 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 2920 TO 4560
PROJECTED ANSWERS: 22 TO 418

L2 11 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 15:22:43 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 3675 TO ITERATE

100.0% PROCESSED 3675 ITERATIONS
SEARCH TIME: 00.00.01

127 ANSWERS

L3 127 SEA SSS FUL L1

=> s l3 and caplus/lc

45300192 CAPLUS/LC

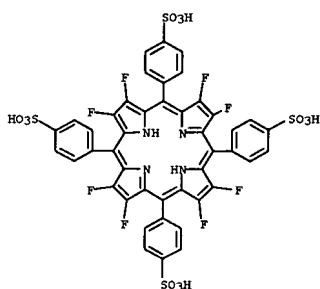
L4 122 L3 AND CAPLUS/LC

=> s l3 not l4

L5 5 L3 NOT L4

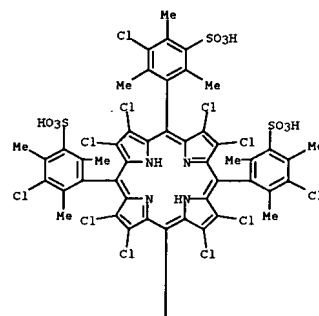
=> d l5 1-5

L5 ANSWER 1 OF 5 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 756473-32-2 REGISTRY
 ED Entered STN: 04 Oct 2004
 CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octafluoro-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis- (9CI) (CA INDEX NAME)
 MF C44 H22 F8 N4 O12 S4
 CI COM
 SR CA



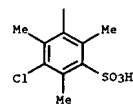
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 2 OF 5 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 738554-86-4 REGISTRY
 ED Entered STN: 03 Sep 2004
 CN Benzenesulfonic acid, 3,3',3'',3'''-(2,3,7,8,12,13,17,18-octachloro-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis[5-chloro-2,4,6-trimethyl- (9CI) (CA INDEX NAME)
 MF C56 H42 Cl12 N4 O12 S4
 CI COM
 SR CA

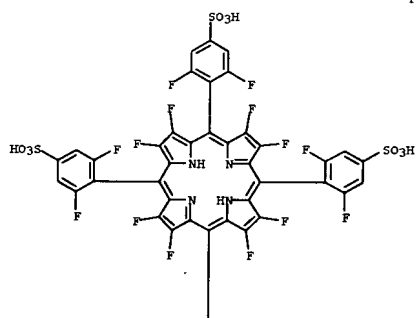


PAGE 1-A

PAGE 2-A

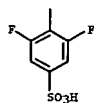


L5 ANSWER 3 OF 5 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 689215-74-5 REGISTRY
 ED Entered STN: 03 Jun 2004
 CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octafluoro-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis(3,5-difluoro- (9CI) (CA INDEX NAME)
 MF C44 H14 F16 N4 O12 S4
 CI COM
 SR CA

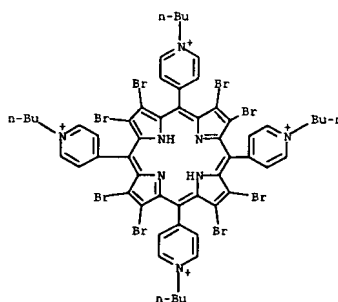


PAGE 1-A

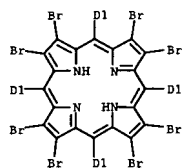
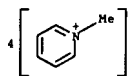
PAGE 2-A



L5 ANSWER 4 OF 5 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 432028-74-5 REGISTRY
 ED Entered STN: 19 Jun 2002
 CN Pyridinium, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis[1-butyl- (9CI) (CA INDEX NAME)
 MF C56 H54 Br8 N8
 CI COM
 SR CA



L5 ANSWER 5 OF 5 REGISTRY COPYRIGHT 2005 ACS on STN
 RN 206349-59-9 REGISTRY
 ED Entered SIN: 04 Jun 1998
 CN Pyridinium, (2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis[1-methyl- (9CI) (CA INDEX NAME)
 MF C44 H30 Br8 N8
 CI IDS, COM
 SR CA



=> fil caplus		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	175.99	176.20

FILE 'CAPLUS' ENTERED AT 15:24:00 ON 01 APR 2005
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FILE COVERS 1907 - 1 Apr 2005 VOL 142 ISS 15
 FILE LAST UPDATED: 31 Mar 2005 (20050331/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 15:22:16 ON 01 APR 2005)

FILE 'REGISTRY' ENTERED AT 15:22:23 ON 01 APR 2005

L1	STRUCTURE UPLOADED
L2	11 S L1
L3	127 S L1 FULL
L4	122 S L3 AND CAPLUS/LC
L5	5 S L3 NOT L4

FILE 'CAPLUS' ENTERED AT 15:24:00 ON 01 APR 2005

=> s l4

L6	148 L4
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=> d ibib abs histr l6 1-148

'HISTR' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'

The following are valid formats:

ABS	-----	GI and AB
ALL	-----	BIB, AB, IND, RE
APPS	-----	AI, PRAI
BIB	-----	AN, plus Bibliographic Data and PI table (default)
CAN	-----	List of CA abstract numbers without answer numbers
CBIB	-----	AN, plus Compressed Bibliographic Data
DALL	-----	ALL, delimited (end of each field identified)
DMAX	-----	MAX, delimited for post-processing
FAM	-----	AN, PI and PRAI in table, plus Patent Family data
FBIB	-----	AN, BIB, plus Patent FAM

IND ----- Indexing data
 IPC ----- International Patent Classifications
 MAX ----- ALL, plus Patent FAM, RE
 PATS ----- PI, SO
 SAM ----- CC, SX, TI, ST, IT
 SCAN ----- CC, SX, TI, ST, IT (random display, no answer numbers;
 SCAN must be entered on the same line as the DISPLAY,
 e.g., D SCAN or DISPLAY SCAN)
 STD ----- BIB, IPC, and NCL

 IABS ----- ABS, indented with text labels
 IALL ----- ALL, indented with text labels
 IBIB ----- BIB, indented with text labels
 IMAX ----- MAX, indented with text labels
 ISTD ----- STD, indented with text labels

 OBIB ----- AN, plus Bibliographic Data (original)
 OIBIB ----- OBIB, indented with text labels

 SBIB ----- BIB, no citations
 SIBIB ----- IBIB, no citations

 HIT ----- Fields containing hit terms
 HITIND ----- IC, ICA, ICI, NCL, CC and index field (ST and IT)
 containing hit terms
 HITRN ----- HIT RN and its text modification
 HITSTR ----- HIT RN, its text modification, its CA index name, and
 its structure diagram
 HITSEQ ----- HIT RN, its text modification, its CA index name, its
 structure diagram, plus NTE and SEQ fields
 FHITSTR ----- First HIT RN, its text modification, its CA index name, and
 its structure diagram
 FHITSEQ ----- First HIT RN, its text modification, its CA index name, its
 structure diagram, plus NTE and SEQ fields
 KWIC ----- Hit term plus 20 words on either side
 OCC ----- Number of occurrence of hit term and field in which it occurs

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of formats include: TI; TI,AU; BIB,ST; TI,IND; TI,SO. You may specify the format fields in any order and the information will be displayed in the same order as the format specification.

All of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR, FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC to view a specified Accession Number.
 ENTER DISPLAY FORMAT (BIB):end

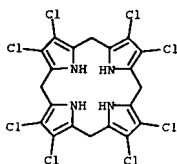
=> d ibib abs hitstr 1-148

L6 ANSWER 1 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2004:925092 CAPLUS
 DOCUMENT NUMBER: 141:349685
 TITLE: Density functional theory studies of β -substituent effect on conformational preference and anion binding ability of calix[4]pyrroles
 AUTHOR(S): Wang, Di-Fei; Wu, Yundong
 CORPORATE SOURCE: Department of Chemistry, The Hong Kong University of Science & Technology, Hong Kong, Peop. Rep. China
 SOURCE: ARKIVOC (Gainesville, FL, United States) (2004), (9), 96-110
 CODEN: AGFUAR
 URL: http://www.arkat-usa.org/ark/journal/2004/I09_Yuan/CY-1155L/CY-1155L.pdf
 PUBLISHER: Arkat USA Inc.
 DOCUMENT TYPE: Journal; (online computer file)
 LANGUAGE: English

AB The conformational features and anion-binding properties of a series of β -octasubstituted calix[4]pyrroles have been investigated by the BLYP method of d. functional theory with the 6-31+G** basis set both in the gas phase and in CH2Cl2 solution. The calcs. demonstrated that adjusting the electronic properties of β -substituents on the pyrrole rings do change the anion-binding ability of calix[4]pyrroles. With the BLYP/6-31+G** method in CH2Cl2 solution, the relative binding energies follow the order of electron withdrawing abilities of the substituents, i.e. CN (18 kcal/mol) >> Cl (7 kcal/mol) > Br (4 kcal/mol) > H (0 kcal/mol). Calcs. also indicate that the energy difference between the most stable 1,3-alternate conformation and the least stable cone-conformation that is for anion-binding is increased by electron-withdrawing β -substituents CN, Cl, and Br. Further anal. on dipyrromethane models reveals that the destabilization of the cone-conformation is mainly caused by electrostatic interactions between the β -substituents on the adjacent pyrrole rings. Our results thus provide useful information for designing stronger and more efficient calix[4]pyrrole-based anion binding receptors.

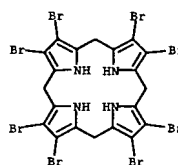
IT 777096-94-3 777096-95-4 777097-11-7
 777097-12-8
 RL: PRP (Properties)
 (DFT studies of β -substituent effect on conformational preference and anion binding ability of calix[4]pyrroles)

RN 777096-94-3 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20,22,24-hexahydro- (9CI) (CA INDEX NAME)

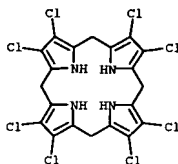


RN 777096-95-4 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20,22,24-hexahydro- (9CI) (CA INDEX NAME)

L6 ANSWER 1 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

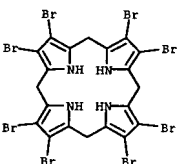


RN 777097-11-7 CAPLUS
 CN Fluoride, compd. with 2,3,7,8,12,13,17,18-octachloro-5,10,15,20,22,24-hexahydro-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)



● F⁻

RN 777097-12-8 CAPLUS
 CN Fluoride, compd. with 2,3,7,8,12,13,17,18-octabromo-5,10,15,20,22,24-hexahydro-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)



● F⁻

L6 ANSWER 1 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN

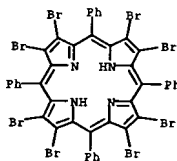
ACCESSION NUMBER: 2004:598751 CAPLUS
 DOCUMENT NUMBER: 141:266257
 TITLE: Conformational analysis of octa- and tetrabromo tetraphenylporphyrins and their Ni(II) and Tb(III) complexes
 AUTHOR(S): Gruden-Pavlovic, Maja; Grubisic, Sonja; Niketic, Svetozar R.
 CORPORATE SOURCE: Belgrade, YU-11001,
 SOURCE: Journal of Inorganic Biochemistry (2004), 98(8), 1293-1302
 CODEN: JIBIDJ; ISSN: 0162-0134
 PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Mol. mechanics (MM) calcs. were used to analyze the puckering of metalloporphyrins as a function of metal ion size and the position of substituents on the porphyrin periphery, on a three series of octa- and tetrabromo tetraphenylporphyrins: without metal, and with Ni(II), and Tb(III) as representative small and large metal ions, resp. Mol. energy optimization calcs. were carried out using the Consistent Force Field (CFF) program, with the parameters developed previously and new parameters for bromine atom. Normal-coordinate structural decomposition (NSD) anal.

was performed on the equilibrium structures obtained by MM calcs. The conformers are also stereochem. characterized, compared with available X-ray structures and with the conformers obtained in our previous MM study using chloro instead of bromo β -pyrrole substituents.

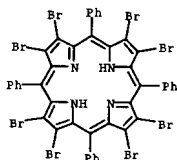
IT 131214-86-3
 RL: PRP (Properties)
 (conformational anal. of octa- and tetrabromo tetraphenylporphyrins and their Ni(II) and Tb(III) complexes)

RN 131214-86-3 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



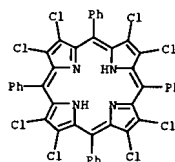
REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2004:501429 CAPLUS
 DOCUMENT NUMBER: 142:287404
 TITLE: Physical-chemical properties of tetraphenylporphyrin, its octasubstituents, and complexes with metals in the ground and excited states
 AUTHOR(S): Kuznetsova, R. T.; Savenkova, N. S.; Mayer, G. V.; Shatunov, P. A.; Semeikin, A. S.
 CORPORATE SOURCE: V.D. Kuznetsov Siberian Physical-Technical Institute, Tomsk State University, Tomsk, Russia
 SOURCE: Atmospheric and Oceanic Optics (2004), 17(2-3), 149-155
 CODEN: AOCEK; ISSN: 1024-8560
 PUBLISHER: Institute of Atmospheric Optics
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The ability of limiting powerful laser radiation (5400 MW/cm²) by solns. of tetraphenylporphyrin (TPP) and its derivs., as well as spectral-luminescent and photochem. properties of these mols. at their excitation to different electronic states by radiation of different wavelength and intensity is studied. The quantum yields of fluorescence from S1 and S_n excited states and in some cases, the quantum yields and features of phototransformations under exposure to powerful laser radiation were determined
 IT 131214-86-3, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenylporphyrin
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
 (Phys.-chemical properties of)
 RN 131214-86-3 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-(9CI) (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2004:484631 CAPLUS
 DOCUMENT NUMBER: 141:184088
 TITLE: Perhalogenated porphyrinic derivatives with indium and thallium: the X-ray structures of (β-C14TPP)Tl(Cl), (β-C14TPP)In(Cl) and (TpFTPP)Tl(Cl)
 AUTHOR(S): Raptopoulou, Catherine; Daphnomili, Dimitra; Karamalides, Athanasios; Di Vaira, Massimo; Terzis, Aris; Coutsolelos, Athanasios G.
 CORPORATE SOURCE: Demokritos, NCSR, Athens, 15310, Greece
 SOURCE: Polyhedron (2004), 23(10), 1777-1784
 CODEN: PLYHDE; ISSN: 0277-5387
 PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The synthesis and spectroscopic characterization of (Porph)M(Cl) where H₂Porph are TpPPP (tetrakis(perfluorophenyl)porphyrin), TPpP (tetrakis(4-pyridyl)porphyrin), β-C14TPP (tetra-β-chlorotetraphenylporphyrin), β-C18TPP (octa-β-chlorotetraphenylporphyrin), β-Br4TPP (tetra-β-bromotetraphenylporphyrin), and M = In or Tl are reported. UV-visible and NMR spectroscopies of the title complexes confirm the proposed mol. formula and are described extracting all plausible information. The study is completed by three x-ray structures of (β-C14TPP)Tl(Cl), (β-C14TPP)In(Cl) and (TpFTPP)Tl(Cl). Compds. (β-C14TPP)Tl(Cl) and (β-C14TPP)In(Cl) are isostructural and they were treated in a similar way. The chloride substituents on the porphyrin core are disordered in both compds. and they were refined anisotropically with occupation factors free to vary. The porphyrin core is saddle distorted while there is no twist distortion as judged by the large values of the dihedral angles formed between the Ph rings and the C20N4 mean plane. In (TpFTPP)In(Cl), the dihedral angles between the pentafluorophenyl rings and C20N4 are very close to the ideal value of 90°.
 IT 120644-25-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reactant for preparation of indium and thallium porphyrin complexes)
 RN 120644-25-9 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-(9CI) (CA INDEX NAME)

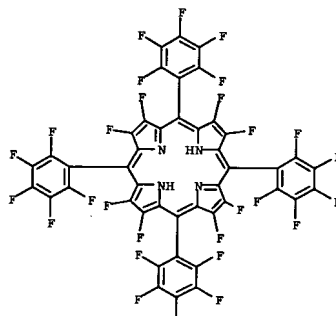


REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2004:400569 CAPLUS
 DOCUMENT NUMBER: 141:133068
 TITLE: Electronic Spectroscopy, Photophysical Properties, and Emission Quenching Studies of an Oxidatively Robust Perfluorinated Platinum Porphyrin
 AUTHOR(S): Lai, Siu-Wai; Hou, Yuan-Jun; Che, Chi-Ming; Pang, Hei-Leung; Wong, Kwok-Yin; Chang, Chi K.; Zhu, Nianying
 CORPORATE SOURCE: Department of Chemistry and Open Laboratory of Chemical Biology of the Institute of Molecular Technology for Drug Discovery and Synthesis, The University of Hong Kong, Hong Kong, Peop. Rep. China
 SOURCE: Inorganic Chemistry (2004), 43(12), 3724-3732
 CODEN: INOCAL; ISSN: 0020-1669
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 141:133068
 AB The highly electron-deficient, β-octafluorinated meso-tetrakis(pentafluorophenyl)porphyrin (H₂F₂₈TPP) was metalated with Pt to afford the oxidatively robust luminophore [PtF₂₈TPP], and its x-ray structure shows that the porphyrin core exists in a slightly saddle-shaped conformation. The absorption spectrum of [PtF₂₈TPP] in CH₂Cl₂ displays a near-UV Soret band (B) at 383 nm and two visible Q(1,0) and Q(0,0) bands at 501 and 533 nm, resp. These absorption bands of [PtF₂₈TPP] are blue-shifted from those in [PtF₂₀TPP] (390, 504, and 538 nm, resp.) and [PtTPP] (401, 509, and 539 nm, resp.). Excitation of [PtF₂₈TPP] in CH₂Cl₂ at the Soret or Q(1,0) or Q(0,0) band gave a phosphorescence with peak maximum at 650 nm (lifetime = 5.8 μs) and a weak shoulder at 712 nm. Both the emission lifetime and quantum yield vary with solvent polarity, and plots of ε vs. EK and Φ vs. EK (EK is the empirical solvent polarity parameter based on the hypsochromic shift of the longest wavelength absorption of the [Mo(CO)₄((C₅H₄N)HC:NCH₂C₆H₅)] complex) with increasing solvent polarity show linear correlation, indicating that the emission is sensitive to the local environment/medium. Electrochem. studies on [PtF₂₈TPP] by cyclic voltammetry showed no porphyrin-centered oxidation at potential ≤ 1.5 V vs. Ag/AgNO₃, demonstrating that [PtF₂₈TPP] is more resistant toward oxidation than [PtF₂₀TPP] (E1/2 = 1.33 V) and [PtTPP] (E1/2 = 0.97 V). The porphyrin-centered reduction of [PtF₂₈TPP] occurs at -0.75 and -1.18 V, which is anodically shifted from those at -1.06 and -1.55 V in [PtF₂₀TPP], and -1.51 V in [PtTPP], resp. The excited-state reduction potential of [PtF₂₈TPP] is 1.49 V vs. Ag/AgNO₃.
 Over 97% of the emission intensity of [PtF₂₈TPP] was retained after irradiation with a high power H₂ arc lamp (500 W) for 14 h, compared to 90% and 12% for [PtF₂₀TPP] and [PtTPP], resp.; hence, [PtF₂₈TPP] exhibits superior photostability. Quenching of the emission of [PtF₂₈TPP] by O₂, alc., catechol, and butylamine reveals that [PtF₂₈TPP] is an oxidatively robust material with medium-sensitive photoluminescence properties.
 IT 121399-88-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reactant for preparation of platinum perfluorinated porphyrin complex)
 RN 121399-88-0 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 5 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

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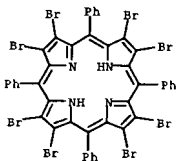
PAGE 2-A

REFERENCE COUNT: 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 6 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2004:356835 CAPLUS
 DOCUMENT NUMBER: 141:359806
 TITLE: Highly brominated porphyrins: synthesis, structure and their properties
 AUTHOR(S): Bhayappa, Puttalah; Purushothaman, Bhavana; Vittal, Jagadees J.
 CORPORATE SOURCE: Department of Chemistry, Indian Institute of Technology-Madras, Chennai, 600 036, India
 SOURCE: Journal of Porphyrins and Phthalocyanines (2003), 7(9 & 10), 682-692
 CODEN: JPPHFZ; ISSN: 1088-4246
 PUBLISHER: Society of Porphyrins & Phthalocyanines
 DOCUMENT TYPE: Journal
 LANGUAGE: English

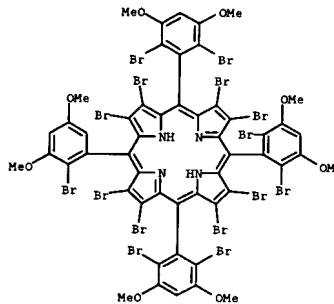
AB This article reports the 1st perbromination of β -pyrrole and meso-Ph groups of the 5,10,15,20-tetrakis(3',5'-dimethoxyphenyl)porphinatocopper(II) to generate highly brominated porphyrin, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2',6'-dibromo-3',5'-dimethoxyphenyl)-porphinatocopper(II), CuT(3',5'-DMP)PBr16 complex. Its crystal structure exhibited unusual five-coordination geometry with saddle shaped conformation of the porphyrin core. H2T(3',5'-DMP)PBr16 and its metal complexes exhibited large anodic shift of oxidation potentials with marginal changes in reduction potentials relative to their corresponding octabromotetraphenylporphyrin, MTPPBr8 derivs. The enhanced electron deficiency of the ZnT(3',5'-DMP)PBr16 complex was probed by axial ligation of various Lewis bases with differing pKa values. The ZnT(3',5'-DMP)PBr16 complex exhibited decrease in equilibrium consts. for the ligation of bases relative to sterically unhindered ZnTPPBr8. This was ascribed to the sterics induced by the bulky ortho-bromo Ph substituents that prevents the facile binding of Lewis bases to the Zn(II)-center.

IT 131214-86-3
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
 (cyclic voltammetry of)
 RN 131214-86-3 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

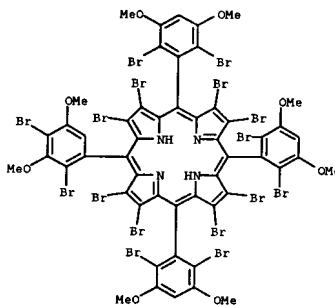


IT 775318-93-9P 775318-94-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 775318-93-9 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5-(2-bromo-3,5-dimethoxyphenyl)-10,15,20-tris(2,6-dibromo-3,5-dimethoxyphenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 6 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

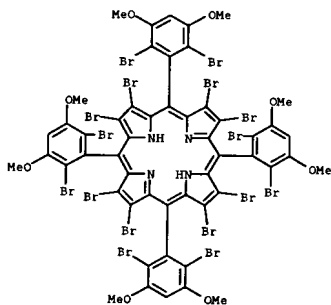


RN 775318-94-0 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5-(2,4-dibromo-3,5-dimethoxyphenyl)-10,15,20-tris(2,6-dibromo-3,5-dimethoxyphenyl)- (9CI) (CA INDEX NAME)



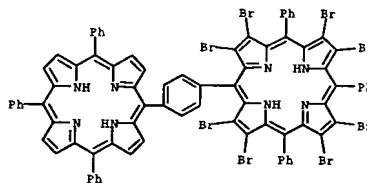
IT 775318-89-3P
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
 (preparation, cyclic voltammetry and reactant for preparation of nickel and zinc highly brominated porphyrin complexes)

L6 ANSWER 6 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
 RN 775318-89-3 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,6-dibromo-3,5-dimethoxyphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 111 THERE ARE 111 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 7 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2004:356825 CAPLUS
 DOCUMENT NUMBER: 141:314040
 TITLE: Synthesis and electrochemical investigation of covalently linked porphyrin dimers containing a β -brominated subunit. Crystal structure of H2(tripp-tpb(Br8))H2
 AUTHOR(S): Ou, Zhongping; Tagliatesta, Pietro; Senge, Mathias O.; Shao, Jiaqun; Kadish, Karl M.
 CORPORATE SOURCE: Department of Chemistry, University of Houston, Houston, TX, 77204-5003, USA
 SOURCE: Journal of Porphyrins and Phthalocyanines (2003), 7(9 & 10), 595-609
 CODEN: JPPHFZ; ISSN: 1088-4246
 PUBLISHER: Society of Porphyrins & Phthalocyanines
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Ten meso-tetraphenyl-porphyrin-type hetero-dimers containing a partly or completely β -brominated subunit were synthesized and characterized by UV-visible spectroscopy, cyclic voltammetry and spectro-electrochem., showing the presence of low electronic interactions between the two subunits. The investigated compds. are represented as M[tripp-tpb(Br4)]M and M[tripp-tpb(Br8)]M (M = 2H, Zn, Ni, Co and Cu) where tripp-tpb(Br4) is the tetra-anion of 1-[5-(10,15,20-triphenyl-porphyrinyl)]-4-[10-(2,3,12,13-tetra-bromo-porphyrinyl)]-benzene and tripp-tpb(Br8) is the tetra-anion of 1-[5-(10,15,20-triphenyl-porphyrinyl)]-4-[10-(2,3,7,8,12,13,17,18-octabromo-porphyrinyl)]-benzene. One of the synthesized dimers, H2(tripp-tpb(Br8))H2, was characterized by a single-crystal X-ray investigation.
 IT 552887-02-2P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (synthesis, crystal structure, cyclic voltammetry, and electrochem. investigation of covalently linked porphyrin dimers containing a β -brominated subunit)
 RN 552887-02-2 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15-triphenyl-20-[4-(10,15,20-triphenyl-21H,23H-porphin-5-yl)phenyl]- (9CI) (CA INDEX NAME)

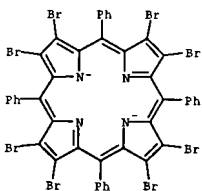


REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 8 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2004:354172 CAPLUS
 DOCUMENT NUMBER: 141:106158
 TITLE: Theoretical AM1 study of acidity of porphyrins, azaporphyrins and porphyrazines
 AUTHOR(S): Stuzhin, Pavel A.
 CORPORATE SOURCE: Department of Organic Chemistry, Ivanovo State University of Chemical Technology, Ivanovo, 153460, Russia
 SOURCE: Journal of Porphyrins and Phthalocyanines (2003), 7(11 & 12), 813-832
 CODEN: JPPHFZ; ISSN: 1088-4246
 PUBLISHER: Society of Porphyrins & Phthalocyanines
 DOCUMENT TYPE: Journal
 LANGUAGE: English

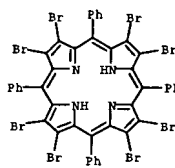
AB The structure-acidity relationship in the series of non-substituted, meso- or β -substituted and β,β -annulated porphyrins and porphyrazines have been studied using the AM1 method with UHF basis set. With this purpose, heats of formation have been determined for the geometry optimized structures of the free base macrocycles and corresponding monoanions and dianions formed by deprotonation. Calculated first deprotonation enthalpy values show correlation with available exptl. pK_a values and can be used for prediction of acidity. For porphyrazines bearing electron-withdrawing substituents or π -deficient annulated heteroarenes the dianions have lower heats of formation than the corresponding neutral species and such porphyrazines are easily deprotonated upon dissoln. in basic solvents (pyridine, DMF). For porphyrazines with annulated 5-member heteroarenes it is predicted that deprotonation of peripheral NH groups should occur more easily than deprotonation of the internal NH groups. The influence of different types of annulation of 5- and 6-membered heteroarenes to the porphyrazine core on the stability of the macrocyclic system and its acidity are also discussed.

IT 717911-35-8
 RL: PRP (Properties)
 (dianion, formation enthalpy; theor. AM1 structure-acidity study of porphyrins, azaporphyrins and porphyrazines)
 RN 717911-35-8 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-, ion(2-) (SCI) (CA INDEX NAME)

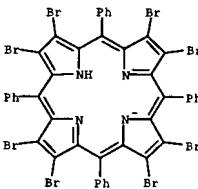


IT 131214-86-3
 RL: PRP (Properties)
 (formation enthalpy and deprotonation enthalpy; theor. AM1 structure-acidity study of porphyrins, azaporphyrins and porphyrazines)

L6 ANSWER 8 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
 RN 131214-86-3 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-, ion(1-) (SCI) (CA INDEX NAME)



IT 717911-25-6
 RL: PRP (Properties)
 (monoanion, formation enthalpy; theor. AM1 structure-acidity study of porphyrins, azaporphyrins and porphyrazines)
 RN 717911-25-6 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-, ion(1-) (SCI) (CA INDEX NAME)

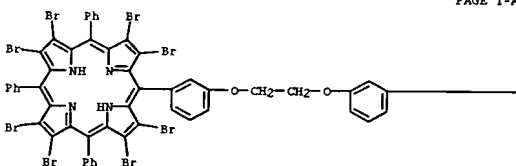


REFERENCE COUNT: 65 THERE ARE 65 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 9 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2004:337463 CAPLUS
 DOCUMENT NUMBER: 141:342314
 TITLE: Covalently linked bisporphyrins bearing tetraphenylporphyrin and perbromoporphyrin units: synthesis and their properties
 AUTHOR(S): Bhyrappa, Puttaiah; Krishnan, V.
 CORPORATE SOURCE: Department of Chemistry, Indian Institute of Technology - Madras, Chennai, 600 036, India
 SOURCE: Journal of Chemical Sciences (Bangalore, India) (2004), 116(2), 71-78
 CODEN: JCSBES
 PUBLISHER: Indian Academy of Sciences
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB A series of covalently linked bisporphyrins bearing meso-tetraphenylporphyrin (TPP) and octabromotetraphenylporphyrin (OBTTP) units have been synthesized and characterized. Electrochem. studies on these bisporphyrins showed an anodic shift (.apprx. 30-60 mV) of the TPP unit and a cathodic shift (.apprx. 40-80 mV) of OBTTP in redox potentials. Further, steady-state fluorescence studies on bisporphyrins indicated dramatic decrease in fluorescence quantum yields of the TPP moiety. Electrochem. redox and fluorescence data seem to suggest the possible existence of intramol. interactions in these bisporphyrins.

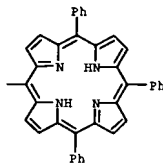
IT 770714-96-0P
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
 (synthesis, electrochem. redox, and fluorescence properties of covalently linked bisporphyrins and their metal complexes bearing tetraphenylporphyrin and perbromoporphyrin)
 RN 770714-96-0 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15-triphenyl-20-[3-{2-(10,15,20-triphenyl-21H,23H-porphin-5-yl)phenoxy}ethoxy]phenyl]- (SCI) (CA INDEX NAME)



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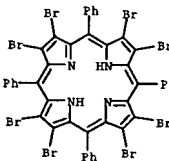
L6 ANSWER 9 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

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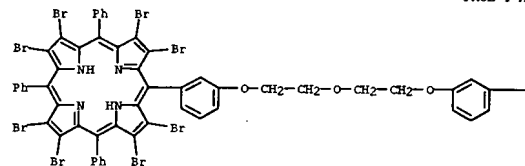
IT 131214-86-3P 770715-01-0P
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
 (synthesis, electrochem. redox, and fluorescence properties of covalently linked bisporphyrins and their metal complexes bearing tetraphenylporphyrin and perbromoporphyrin)

RN 131214-86-3 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-, ion(1-) (SCI) (CA INDEX NAME)

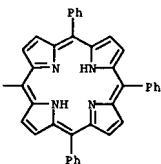


RN 770715-01-0 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15-triphenyl-20-[3-{2-(10,15,20-triphenyl-21H,23H-porphin-5-yl)phenoxy}ethoxy]ethoxy]phenyl]- (SCI) (CA INDEX NAME)

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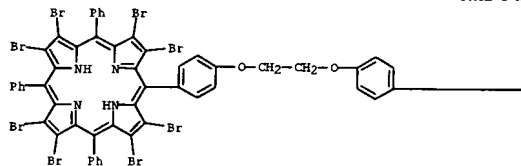


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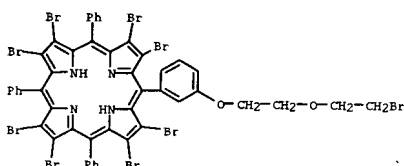


IT 770714-95-9P
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (synthesis, electrochem. redox, and fluorescence properties of covalently linked bisporphyrins and their metal complexes bearing tetraphenylporphyrin and perbromoporphyrin)
 RN 770714-95-9 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15-triphenyl-20-[4-(2-bromoethoxy)ethoxy]phenyl-10,15,20-triphenyl- (9CI) (CA INDEX NAME)

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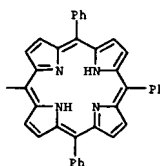


RN 770714-94-8 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5-[3-(2-(2-bromoethoxy)ethoxy)phenyl]-10,15,20-triphenyl- (9CI) (CA INDEX NAME)

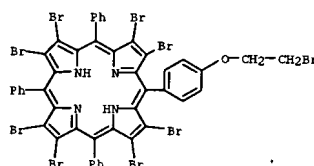


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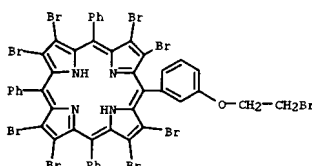
PAGE 1-B



IT 213414-00-7P 770714-93-7P 770714-94-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (synthesis, electrochem. redox, and fluorescence properties of covalently linked bisporphyrins and their metal complexes bearing tetraphenylporphyrin and perbromoporphyrin)
 RN 213414-00-7 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5-[4-(2-bromoethoxy)phenyl]-10,15,20-triphenyl- (9CI) (CA INDEX NAME)



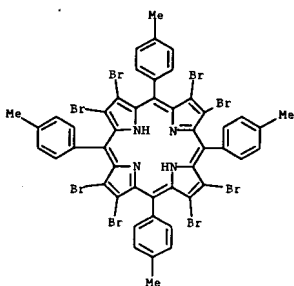
RN 770714-93-7 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5-[3-(2-bromoethoxy)phenyl]-10,15,20-triphenyl- (9CI) (CA INDEX NAME)



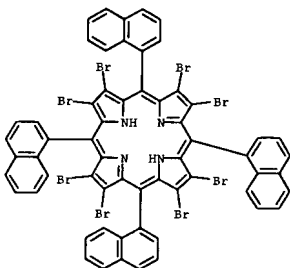
ACCESSION NUMBER: 2003:781478 CAPLUS
 DOCUMENT NUMBER: 140:76935
 TITLE: Solvent effects on some new meso-aryl substituted octabromoporphyrins
 AUTHOR(S): George, Regimol G.; Padmanabhan, M.
 CORPORATE SOURCE: School of Chemical Sciences, Mahatma Gandhi University, Kottayam, 686 560, India
 SOURCE: Proceedings - Indian Academy of Sciences, Chemical Sciences (2003), 115(4), 263-271
 CODEN: FIADMD; ISSN: 0253-4134
 PUBLISHER: Indian Academy of Sciences
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB A series of porphyrins with tolyl and naphthyl substituents at the meso positions, their octabromo derivs. (OBP) with Br substituents at β -pyrrole positions are synthesized and characterized by chemical anal., ¹H NMR and electronic spectral studies. It is seen that all the OBPs exhibit pronounced red shifts in both the Soret and Q bands of their electronic spectra compared to their non-brominated form in various polar and nonpolar solvents, the energy difference $\Delta E_{Soret-Q}$ being in the range 2300-2700 cm⁻¹. The high energy B band of naphthyl porphyrins (both brominated and nonbrominated) are found to be more red-shifted than that of tolyl porphyrins, owing to the noticeable mesomeric effect of the naphthyl groups. Detailed spectral studies reveal that while none of the nonbrominated porphyrin show solvent-dependent change in their B and Q bands, all the OBPs manifest significant shifts depending on the nature of solvents. Solvent-solute interaction can be considered to be of strong dipole-dipole nature for OBPs with polar solvents and of $\pi-\pi$ type with aromatic non-polar solvents. In the brominated form we find two categories of porphyrins exhibiting distinctly different absorption phenomena in aromatic solvents. The OBPs having meso-groups not shielding the porphyrin π -framework exhibit addnl. absorption peaks (split Soret peaks and broadened Q bands) in some aromatic solvents. This could be explained in terms of $\pi-\pi$ type donor-acceptor (DA) complex formation between such bromoporphyrins (acceptor) and the aromatic solvent mol's. (donor) that is not possible for OBPs that have bulky meso groups that block the approach of aromatic solvent mol's. close to the porphyrin framework.

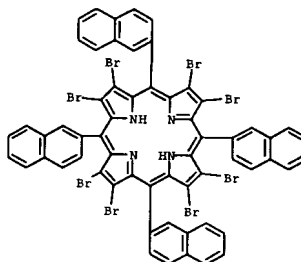
IT 182423-35-4 640730-26-3 640730-27-4
 640730-28-5 640730-29-6
 RL: PRP (Properties)
 (solvent effects on absorption spectra of meso-aryl substituted octabromoporphyrins)
 RN 182423-35-4 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(4-methylphenyl)- (9CI) (CA INDEX NAME)



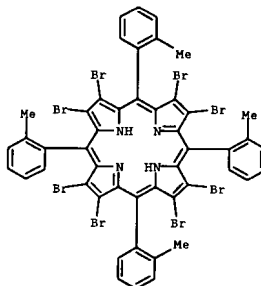
RN 640730-26-3 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetra-1-naphthalenyl- (9CI) (CA INDEX NAME)



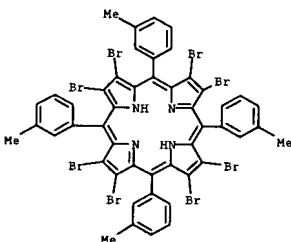
RN 640730-27-4 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetra-2-naphthalenyl- (9CI) (CA INDEX NAME)



RN 640730-28-5 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2-methylphenyl)- (9CI) (CA INDEX NAME)

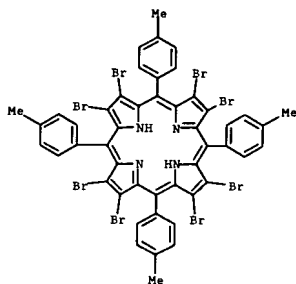


RN 640730-29-6 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(3-methylphenyl)- (9CI) (CA INDEX NAME)

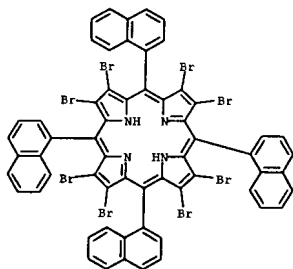


REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

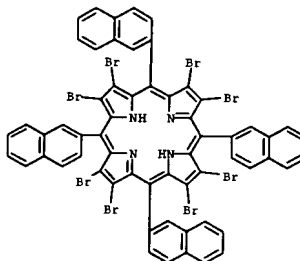
ACCESSION NUMBER: 2003:762928 CAPLUS
DOCUMENT NUMBER: 140:103814
TITLE: Studies on some new meso-aryl substituted octabromo-porphyrins and their Zn(II) derivatives
AUTHOR(S): George, Regimol G.; Padmanabhan, M.
CORPORATE SOURCE: School of Chemical Sciences, Mahatma Gandhi University, Kottayam, 686560, India
SOURCE: Polyhedron (2003), 22(23), 3145-3154
CODEN: PLYHDE; ISSN: 0277-5387
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Porphyrins with various tolyl (H2TTHP) and naphthyl substituents (H2TNHP) at the meso-positions, their octabromo derivs. (H2TTBP and H2TNBP) with Br substituents at β -pyrrole positions and also their Zn(II) derivs. were synthesized and characterized by ¹H NMR, electronic, fluorescence and electrochem. studies. These have the meso-carbons bonded to tolyl moieties at ortho-, meta- and para-positions of the tolyl groups and at the α - or β -position of the naphthyl group. For the octabromoporphyrins, pronounced deshielding of NH protons and a moderate shift of meso-aryl protons to a lower δ value are observed compared to their nonbrominated species. The electronic spectra of ZnTTHP and ZnTNHP have almost the same B and Q bands while the B band of their free-base analogs have H2TNHP absorbing at a higher wavelength than H2TTHP. All the octabromo derivs. exhibit a pronounced red shift for both B and Q bands (compared to their nonbrominated forms) and show meso-substituent dependent change in both free-base and metalated forms. The above observations are interpreted in terms of moderate conjugative interaction of the aryl substituent with the π framework and also in terms of energy level reordering which alters the HOMO-LUMO gap. Consistent with the absorption spectral data the emission bands of all the bromoporphyrins also are red shifted considerably. Significant decrement in quantum yield (ϕ_f) was observed for the bromo compds. While the ϕ_f of nonbrominated porphyrins is higher than their Zn(II) derivs. the reverse order is observed for the bromo derivs. The ability of the Zn²⁺ ion to make the bromoporphyrins resistant to distortion by bridging the central cavity can be attributed as the cause for this interesting observation. Cyclic voltammetric studies exhibit characteristic quasi-reversible/irreversible oxidation-reduction features for all the free-bases and Zn(II) derivs. The bromo derivs. however, manifest marginally harder oxidation and very easy reduction features. The data are interpreted in terms of electron withdrawing ability of Br atoms and to reordering of HOMO and LUMO levels due to distortion in the porphyrin ring.
IT 182423-35-4P 640730-26-3P 640730-27-4P 640730-28-5P 640730-29-6P
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent) (preparation, electrochem. properties, metalation with zinc and electronic and fluorescence spectra of meso-tetraaryl substituted octabromoporphyrin)
RN 182423-35-4 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(4-methylphenyl)- (9CI) (CA INDEX NAME)



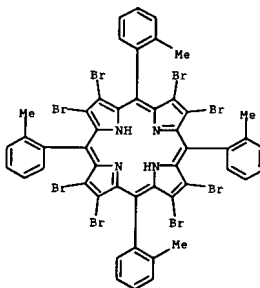
RN 640730-26-3 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetra-1-naphthalenyl- (9CI) (CA INDEX NAME)



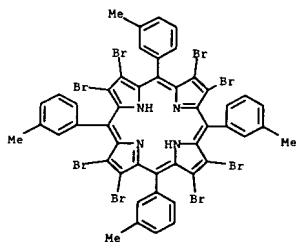
RN 640730-27-4 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetra-2-naphthalenyl- (9CI) (CA INDEX NAME)



RN 640730-28-5 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2-methylphenyl)- (9CI) (CA INDEX NAME)

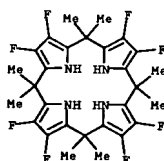


RN 640730-29-6 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(3-methylphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 12 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:623230 CAPLUS
DOCUMENT NUMBER: 139:370552
TITLE: Fluorinated calixpyrroles: anion-binding extractants that reduce the Hofmeister bias
AUTHOR(S): Levitskaia, Tatiana G.; Marquez, Manuel; Sessler, Jonathan L.; Shriver, James A.; Vercouter, Thomas; Moyer, Bruce A.
CORPORATE SOURCE: Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37830-6119, USA
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2003), (17), 2248-2249
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB β -Octafluoro-meso-octamethylcalix[4]pyrrole (I) and β -decafluoro-meso-decamethylcalix[5]pyrrole (II) were found to extract cesium salts of smaller anions (bromide and chloride for I and nitrate for II) as effectively as that of iodide into nitrobenzene (NB) thereby overcoming the Hofmeister bias normally observed for processes of this type.
IT 311804-81-6
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
(cesium salt solvent extn with fluorinated calixpyrroles and attenuation of Hofmeister series)
RN 311804-81-6 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 13 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:563277 CAPLUS
DOCUMENT NUMBER: 139:239081
TITLE: Synthesis and Structural Characterization of Porphyrinic Bredyynes: Geometric and Electronic Effects on Thermal and Photochemical Reactivity
AUTHOR(S): Chandra, Tilak; Kraft, Brian J.; Huffman, John C.; Zaleski, Jeffrey M.
CORPORATE SOURCE: Department of Chemistry and Molecular Structure Center, Indiana University, Bloomington, IN, 47405-7102, USA
SOURCE: Inorganic Chemistry (2003), 42(17), 5158-5172
CODEN: INOCJH; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:239081

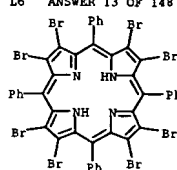
AB The authors report the preparation of 5,10,15,20-tetraphenyl-2,3,7,8,12,13,17,18-octakis(phenylethynyl)porphine and its Ni(II), Zn(II), Mg(II), and Cu(II) complexes, as well as select trimethylsilylphenylethynyl derivs. The X-ray structures of the octakis(phenylethynyl) compds. show systematic deviations from planarity (Ni(II), 0.2851 Å; Zn(II), 0.0304 Å) as a function of the central cation. These geometric distortions are reflected in bathochromic shifts of the Soret and Q bands (Ni(II), 497, 604, and 650 nm; Mg(II), 515, 595, 642, and 705 nm) which loosely correlate with increasing planarity of the structure. Similarly, vibrational modes involving the octa-substituted porphyrin core exhibit shifts to lower frequency as a function of increasing planarity in the solution-state resonance Raman spectra (λ_{exc} = 501.7 nm) of these compds. Analogous trends are also observed in their solid-state electronic and resonance Raman spectra, indicating that the structural distortions within the octakis(phenylethynyl) series are preserved in solution. Comparison of the saddle distortion of the octa-substituted Ni(II) compound with the ruffle/saddle distortions of the pentakis and hexakis Ni(II) derivs. reveals some influence of asym. peripheral substitution on geometric structure. These Ni(II) derivs. also exhibit systematic red shifts in their electronic spectra as a function of the number of conjugated alkyne units (.apprx.13 nm/alkyne), revealing participation of the brediyne units in the electronic ground and excited states. The solid-state Bergman cyclization temps. of the phenylethynyl compds. vary markedly as a function of planarity, and correlate loosely with alkyne termini separation (Ni(PA)8, 4.00 Å, 281°; MgP(PA)8, 3.77 Å, 244°). In solution, both thermal and photochem. activation of the free-base octakis(phenylethynyl) compound lead to formal reduction of the porphyrin backbone via H-atom addition at opposing meso-positions. Generation of a common product suggests that both thermal and photochem. pathways to Bergman cyclization in solution contain significant activation barriers to formation of the 4-Ph diradical intermediate, and under these solution conditions, alternate reaction channels are more thermodynamically favorable.

IT 131214-86-3, 2,3,7,8,12,13,17,18-Octabromo-5,10,15,20-tetraphenylporphine

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of ethynyl-substituted tetraphenylporphines and their magnesium and transition metal complexes)

RN 131214-86-3 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

L6 ANSWER 13 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



REFERENCE COUNT: 100 THERE ARE 100 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L6 ANSWER 14 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:41405 CAPLUS
DOCUMENT NUMBER: 138:409450
TITLE: Optical recording media having super resolution mask layer and method for recording/reading thereof
INVENTOR(S): Sato, Tsutomu; Tomura, Tatsuya; Ueno, Yasunobu
PATENT ASSIGNEE(S): Ricoh Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKKOAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

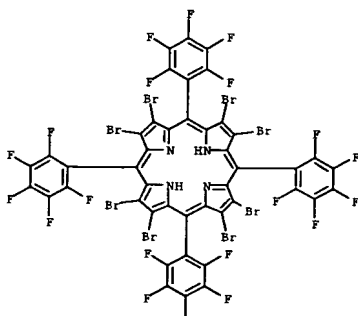
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003157584	A2	20030530	JP 2001-357662	20011122
PRIORITY APPLN. INFO.:			JP 2001-357662	20011122

AB The title optical disk has a recording layer on a substrate, wherein a super resolution mask layer contains dispersed porphyrin derivative and is disposed on the recording layer. The optical disk has data storage d. over the diffraction limit of the pick-up lens.

IT 139944-26-6
RL: TEM (Technical or engineered material use); USES (Uses)
(super resolution mask layer in optical recording media)

RN 139944-26-6 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

PAGE 1-A



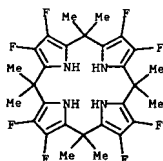
L6 ANSWER 14 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 2-A

L6 ANSWER 15 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:385522 CAPLUS
DOCUMENT NUMBER: 139:100832
TITLE: Single Side Strapping: A New Approach to Fine Tuning the Anion Recognition Properties of Calix[4]pyrroles
AUTHOR(S): Lee, Chang-Hee; Na, Hee-Kyung; Yoon, Dae-Wi; Won, Dong-Hoon; Cho, Won-Seob; Lynch, Vincent M.; Shevchuk, Sergey V.; Sessler, Jonathan L.
CORPORATE SOURCE: Department of Chemistry, Kangwon National University, Chun-Chon, 200-701, S. Korea
SOURCE: Journal of the American Chemical Society (2003), 125(24), 7301-7306
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:100832

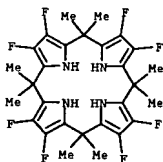
AB Three calix[4]pyrroles bearing m-ocinol-derived diether straps of different lengths on one side of the tetrapyrrolic core were synthesized and characterized. Structural information for an analogous diester bridged strapped system reported previously (Yoon, D. W.; Hwang, H.; Lee, C. H. Angew. Chem., Int. Ed. Engl. 2002, 41, 1757-1759) is also provided as are bromide and chloride anion affinities for all four systems determined by Isothermal Titration Calorimetry (ITC) in acetonitrile. Although both sets of the strapped calix[4]pyrroles displayed enhanced affinities for chloride and bromide anion, differences were seen among the various receptors that support the conclusion that the anion binding ability of calixpyrrole-type systems can be effectively tuned by modifying the length and nature of the bridging straps. In the specific case of the diether systems, the largest chloride affinity was seen with the shortest strap, whereas the largest affinity for bromide anion was recorded in the case of the longest strap. As well as supporting 1H NMR spectroscopic studies, it is postulated that not only cavity size per se, but also the ability of the aryl portion of the strap to serve as a CH H bond donor site are important in regulating the observed anion affinities.

IT 311804-81-6
RL: CFS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(complexation of halide salts; single side strapping approach to fine tuning anion recognition properties of calix[4]pyrroles)
RN 311804-81-6 CAPLUS
CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)



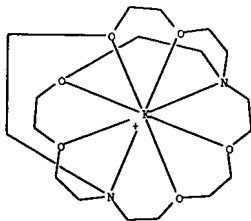
IT 311804-88-3 560094-16-8 560094-21-5

L6 ANSWER 15 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



CM 2

CRN 12569-48-1
CMF C18 H36 K N2 O6 . C1
CCI CCS



● Cl⁻

RN 560094-21-5 CAPLUS
CN 1-Butanaminium, N,N,N-tributyl-, bromide, compd. with 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)

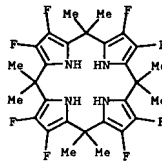
CM 1

CRN 311804-81-6
CMF C28 H28 F8 N4

L6 ANSWER 15 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); FORM (Formation, nonpreparative); PROC (Process)
(single side strapping approach to fine tuning anion recognition properties of calix[4]pyrroles)
RN 311804-88-3 CAPLUS
CN 1-Butanaminium, N,N,N-tributyl-, chloride, compd. with 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)

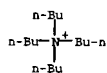
CM 1

CRN 311804-81-6
CMF C28 H28 F8 N4



CM 2

CRN 1112-67-0
CMF C16 H36 N . C1



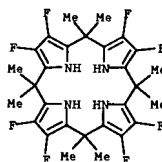
● Cl⁻

RN 560094-16-8 CAPLUS
CN Potassium(1+), (4,7,13,16,21,24-hexaaza-1,10-diazabicyclo[8.8.8]hexacosane-κN1,κN10,κO4,κO7,κO13,κO16,κO21,κO24)-, chloride, compd. with 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)

CM 1

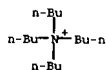
CRN 311804-81-6
CMF C28 H28 F8 N4

L6 ANSWER 15 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



CM 2

CRN 1643-19-2
CMF C16 H36 N . Br



● Br⁻

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2003:290712 CAPLUS
DOCUMENT NUMBER: 139:45848TITLE: Differential substituent effects of β -halogens in water-soluble porphyrins
AUTHOR(S): Biffinger, Justin C.; Sun, Haoran; Nelson, Andrew P.; DiMaggio, Stephen G.

CORPORATE SOURCE: Department of Chemistry, University of Nebraska, Lincoln, NE, USA

SOURCE: Organic & Biomolecular Chemistry (2003), 1(4), 733-736
CODEN: OBCRAK; ISSN: 1477-0520

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:45848

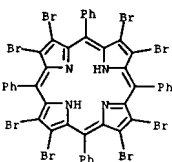
AB The 1st water-soluble β -octafluorinated porphyrins, 5,10,15,20-tetrakis(4-sulfonatophenyl)-2,3,7,8,12,13,17,18-octafluoroporphyrin, 1, and 5,10,15,20-tetrakis(2,6-difluoro-3-sulfonatophenyl)-2,3,7,8,12,13,17,18-octafluoroporphyrin, 2, were prepared and their aqueous aggregation, acid-base, and optical properties were characterized. The porphyrins are tetraanionic at neutral pH (at pH = 3-11 for 1 and pH = 0-9 for 2). Semiempirical (AM1) calcs. provide evidence that somewhat unusual acidity characteristics of the fluorinated compds. (with respect to similar brominated porphyrins) can be rationalized solely from chemical hardness and electronegativity arguments. The large conformational differences seen in the structures of brominated and fluorinated water-soluble porphyrins have little impact upon N-H acidity. Metalation of 1 and 2 with ZnCl₂ yielded the corresponding Zn complexes, which were characterized by optical spectroscopy and electrochem.

IT 131214-86-3, 2,3,7,8,12,13,17,18-Octabromo-5,10,15,20-tetraphenylporphyrin 144811-83-6, 2,3,7,8,12,13,17,18-Octabromo-5,10,15,20-tetraphenylporphyrin 541528-61-4

RL: PRP (Properties)
(energy of gas phase acidities from semiempirical AM1 calcs.)

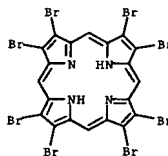
RN 131214-86-3 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



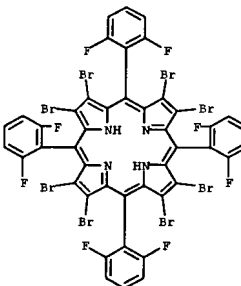
RN 144811-83-6 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo- (9CI) (CA INDEX NAME)



RN 541528-61-4 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,6-difluorophenyl)- (9CI) (CA INDEX NAME)



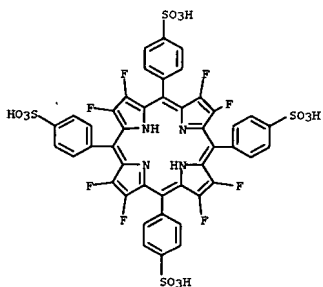
IT 541528-56-7P 541528-57-8P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and complexation with zinc and acidity)

RN 541528-56-7 CAPLUS

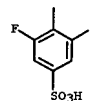
CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octafluoro-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis-, tetrasodium salt (9CI) (CA INDEX NAME)

PAGE 2-A



RN 541528-57-8 CAPLUS

CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octafluoro-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis[3,5-difluoro-, tetrasodium salt (9CI) (CA INDEX NAME)



● 4 Na

IT 541528-60-3P

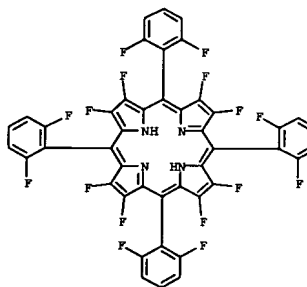
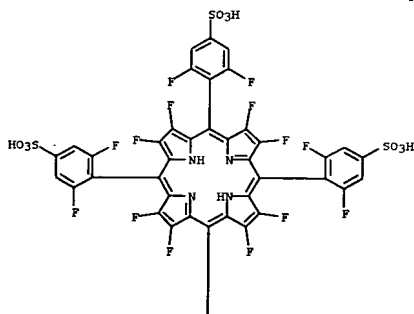
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactant for preparation of

tetrakis(difluorosulfonatophenyl)octafluoroporphyrin)

RN 541528-60-3 CAPLUS

CN 21H,23H-Porphine, 5,10,15,20-tetrakis(2,6-difluorophenyl)-2,3,7,8,12,13,17,18-octafluoro- (9CI) (CA INDEX NAME)

PAGE 1-A

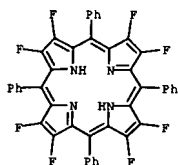


IT 186885-28-9, 2,3,7,8,12,13,17,18-Octafluoro-5,10,15,20-tetraphenylporphyrin

RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(reactant for preparation of tetrakis(sulfonatophenyl)octafluoroporphyrin and energy of gas phase acidities from semiempirical AM1 calcs.)

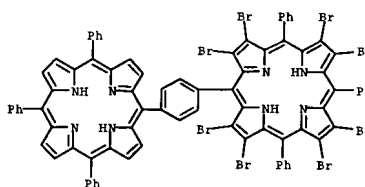
RN 186885-28-9 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



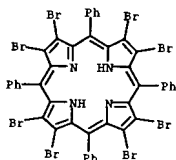
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 17 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2003:243699 CAPLUS
 DOCUMENT NUMBER: 139:92612
 TITLE: Perhalogenated porphyrins as a sink of excitation energy in porphyrin heterodimers
 AUTHOR(S): Venanzi, Mariano; Tagliatesta, Pietro; Pastorini, Alessandra; Mari, Patrizia; Elisei, Fausto; Latterini, Loredana; Kadish, Karl M.
 CORPORATE SOURCE: Dipartimento di Scienze e Tecnologie Chimiche, Univ. Roma-Tor Vergata, Rome, 00133, Italy
 SOURCE: Journal of Porphyrins and Phthalocyanines (2002), 6(9 & 10), 643-652
 CODEN: JPPHFZ; ISSN: 1088-4246
 PUBLISHER: Society of Porphyrins & Phthalocyanines
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The photophysics of a new family of free-base and zinc derivs. of meso-tetraphenylporphyrin heterodimers have been studied by UV-vis absorption, fluorescence and nanosecond flash photolysis techniques. An almost complete (~99%) and directionally controlled transfer of excitation energy from a donor porphyrin moiety was obtained by multiple bromination (four and eight Br substituents in the two series of compds. investigated) on the β -pyrrole positions of the acceptor porphyrin mol. The covalently linked porphyrin dimers populate almost exclusively low energy triplet states because of the extremely efficient intramol. singlet-to-triplet inter system crossing (ISC) process which is enhanced by the multiple heavy atoms substitutions. The nature of the electronic interactions determining the actual relaxation pathway followed by the porphyrin donor-acceptor pair is discussed.
 IT 552887-02-2
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); FRP (Properties); PROC (Process)
 (perhalogenated porphyrins as sink of excitation energy in porphyrin heterodimers)
 RN 552887-02-2 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15-triphenyl-20-[4-(10,15,20-triphenyl-21H,23H-porphin-5-yl)phenyl]- (9CI) (CA INDEX NAME)



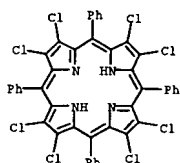
IT 131214-86-3, 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo, 5,10,15,20-Tetraphenyl
 RL: FRP (Properties)
 (perhalogenated porphyrins as sink of excitation energy in porphyrin heterodimers)
 RN 131214-86-3 CAPLUS

L6 ANSWER 17 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 18 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2003:226965 CAPLUS
 DOCUMENT NUMBER: 138:401523
 TITLE: Electronic Absorption and Resonance Raman Signatures of Hyperporphyrins and Nonplanar Porphyrins
 AUTHOR(S): Wasbotten, Ingar H.; Conradie, Jeanet; Ghosh, Abhik
 CORPORATE SOURCE: Institute of Chemistry, Faculty of Science, University of Tromsø, Tromsø, N-9037, Norway
 SOURCE: Journal of Physical Chemistry B (2003), 107(v 15), 3613-3623
 CODEN: JPCBFX; ISSN: 1520-6106
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB We have carried out a broad survey of tetraphenylporphyrin derivs. in relation to their possible hyperporphyrin character. The majority of the free-base tetraphenylporphyrins studied, i.e., TArPH2; Ar = p-X-C6H4, where X = CH3, H, F, CF3, and NO2, when dissolved in trifluoroacetic acid (i.e. when centrally diprotonated), exhibit red-shifted "hyperporphyrin" spectra. The "hyper" features are attributable to phenyl-to-porphyrin charge-transfer transitions. However, certain free-base tetraphenylporphyrins with extremely electron-deficient Ph groups, such as TPFPFH2, do not exhibit hyperporphyrin spectra in trifluoroacetic acid solution. Certain anionic tetraphenylporphyrin derivs. such as T(p-OH-P)PH2 or Ni(T(p-OH-P)P) dissolved in methanolic Bu4NOH also qualify as hyperporphyrins. The hyper transitions in these cases involve charge transfer from anionic phenolate substituents to the neutral porphyrin core. This study also presents a first systematic resonance Raman spectroscopic exploration of hyperporphyrins. Comparison of the Soret-resonant Raman spectra of various normal, hyper-, and hypso-tetraphenylporphyrin derivs. indicates that the former two categories generally exhibit a more intense ν_1 band, which is the fully sym. Cmeso-Opheyl stretching vibration, relative to hypso-porphyrins such as square-planar nickel tetraarylporphyrins. We have also reinvestigated recent reports of large red shifts observed for the electronic spectra of saddled porphyrins in polar solvents, an effect attributed to increased N-H...solvent hydrogen bonding in polar solvents. Interestingly, we find that such solvent-induced red shifts are observed for the relatively electron-deficient porphyrin Br8TPFH2, Cl8TPFH2, and OETNPH2 but not for the relatively electron-rich OETPFH2. Resonance Raman spectra of these saddled porphyrins in different solvents reveal little shift in the high-frequency marker bands, which is consistent with little change in macrocycle conformation with solvent polarity. The observed solvent-induced red shifts in the electronic spectra therefore appear to reflect a largely electronic (as opposed to conformational) effect of N-H...solvent hydrogen bonding in polar solvents. Finally, we also present a chronol. summary of the controversial question as to whether nonplanar deformations are actually responsible for the red-shifted electronic spectra of the majority of nonplanar porphyrins.
 IT 120644-25-9, β -Octachloro-meso-tetraphenylporphyrin
 131214-86-3, β -Octabromo-meso-tetraphenylporphyrin
 RL: PEP (Physical, engineering or chemical process); PYP (Physical process); PROC (Process)
 (electronic absorption and resonance Raman signatures of hyperporphyrins and nonplanar porphyrins)
 RN 120644-25-9 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



RN 131214-86-3 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-
(9CI) (CA INDEX NAME)

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2003:167716 CAPLUS
DOCUMENT NUMBER: 138:347950
TITLE: Unusual Aryl-Porphyrin Rotational Barriers in Peripherally Crowded Porphyrins
AUTHOR(S): Medforth, Craig J.; Haddad, Raid E.; Muzzi, Cinzia M.; Dooley, Neal R.; Jaquinod, Laurent; Shyr, David C.; Nurco, Daniel J.; Olmstead, Marilyn M.; Smith, Kevin M.; Ma, Jian-Guo; Shelton, John A.
CORPORATE SOURCE: Department of Chemistry, University of California, Davis, CA, 95616, USA
SOURCE: Inorganic Chemistry (2003), 42(7), 2227-2241
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:347950

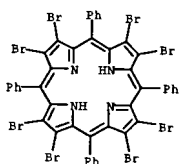
AB Previous studies of 5,10,15,20-tetraarylporphyrins showed that the barrier for meso aryl-porphyrin rotation (AG.dbldag.ROT) varies as a function of the core substituent M and is lower for a small metal (M = Ni) compared to a large metal (M = Zn) and for a dication (M = 4H2+) vs. a free base porphyrin (M = 2H). This was attributed to changes in the nonplanar distortion of the porphyrin ring and the deformability of the macrocycle caused by the core substituent. X-ray crystallog., mol. mechanics (MM) calcs., and variable temperature (VT) 1H NMR spectroscopy

were used to examine the relation between the aryl-porphyrin rotational barrier and the core substituent M in some novel 2,3,5,7,8,10,12,13,15,17,18,20-dodecaarylporphyrins (DARPs), and specifically in some 5,10,15,20-tetraaryl-2,3,7,8,12,13,17,18-octaphenylporphyrins (TAROPPs), where steric crowding of the peripheral groups always results in a very nonplanar macrocycle. X-ray structures of DARPs indicate differences in the nonplanar conformation of the macrocycle as a function of M, with saddle conformations being observed for M = Zn, 2H or M = 4H2+ and saddle and/or ruffle conformations for M = Ni. Variable-temperature NMR studies

show that the effect of protonation in the TAROPPs is to increase AG.dbldag.ROT, which is the opposite of the effect seen for the TARPs, and MM calcs. also predict a strikingly high barrier for the TAROPPs when M = 4H2+. These and other findings suggest that the aryl-porphyrin rotational barriers in the DARPs are closely linked to the deformability of the macrocycle along a nonplanar distortion mode which moves the substituent being rotated out of the porphyrin plane.

IT 131214-86-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(Suzuki coupling reaction with phenylboronic acids)

RN 131214-86-3 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-
(9CI) (CA INDEX NAME)



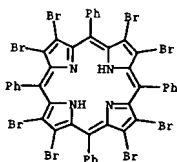
REFERENCE COUNT: 110 THERE ARE 110 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2003:164009 CAPLUS
DOCUMENT NUMBER: 138:344519
TITLE: Effect of a proton-donating solvent on complexation of classical and nonclassical porphyrins in a pyridine medium
AUTHOR(S): Berezin, D. B.; Toldina, O. V.
CORPORATE SOURCE: Russia
SOURCE: Zhurnal Neorganicheskoi Khimii (2002), 47(12), 2075-2081
CODEN: ZNOKAQ; ISSN: 0044-457X
PUBLISHER: MAIK Nauka/Interperiodica Publishing
DOCUMENT TYPE: Journal
LANGUAGE: Russian

AB The inhibiting effect of proton-donating additives (HAc) on the rate of coordination of tetrabenzoporphine (I) and tetraphenyltetrabenzoporphine (I) as well as of N-substituted porphyrins (III and IV) with CuAc2 and ZnAc2 in a pyridine medium is shown. It is also shown that in the compds. I and II, the properties of the NH bond and the reactivity for a given reaction are close to those for nonclassical porphyrins (H2P). The N-substituted porphyrins III et IV do not behave the same way. The inhibition of the coordination reaction in the compound III and IV can be explained by the increase of basicity of the tertiary nitrogen atoms in these mols.

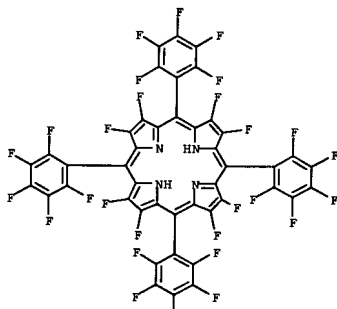
IT 131214-86-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(effect of a proton-donating solvent on complexation of classical and nonclassical porphyrins in a pyridine medium)

RN 131214-86-3 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-
(9CI) (CA INDEX NAME)



L6 ANSWER 21 OF 148 CAPLUS COPYRIGHT 2005 ACS ON STN
 ACCESSION NUMBER: 2003:69802 CAPLUS
 DOCUMENT NUMBER: 138:401522
 TITLE: Perfluorinated meso-aryl-substituted expanded porphyrins
 AUTHOR(S): Shimizu, Soji; Shin, Ji-Young; Furuta, Hiroyuki; Ismael, Rami; Osuka, Atsuhiko
 CORPORATE SOURCE: Department of Chemistry Graduate School of Science, Kyoto University, Kyoto, 606-8502, Japan
 SOURCE: Angewandte Chemie, International Edition (2003), 42(1), 78-82
 CODEN: AIEF5; ISSN: 1433-7851
 PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 138:401522
 AB The title porphyrins were prepared by condensation of perfluorophenol and 3,4-difluoropyrrole and characterized as to structure and conformation by spectral and X-ray crystallog. means.
 IT 121399-88-ODP, ring expanded analogs 121399-88-OP
 RI: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation, conformation and crystal structure of perfluorinated meso-aryl-substituted expanded porphyrins)
 RN 121399-88-0 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

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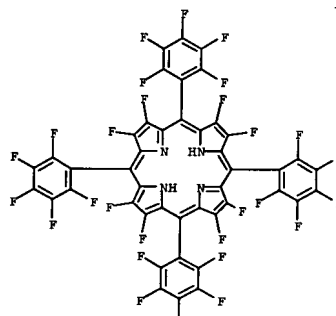


PAGE 2-A

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L6 ANSWER 21 OF 148 CAPLUS COPYRIGHT 2005 ACS ON STN (Continued)
 RN 121399-88-0 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

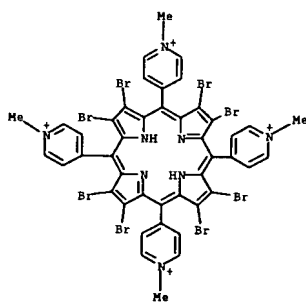


PAGE 2-A

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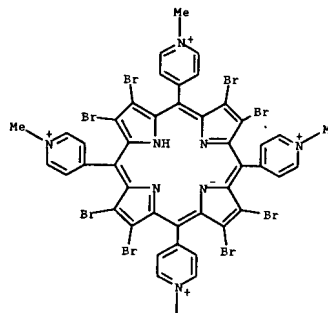
REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 22 OF 148 CAPLUS COPYRIGHT 2005 ACS ON STN
 ACCESSION NUMBER: 2003:66387 CAPLUS
 DOCUMENT NUMBER: 138:276888
 TITLE: Kinetics of the reactions of divalent copper, zinc, cobalt, and nickel with a deformed water soluble centrally monoprotoporphyrin
 AUTHOR(S): Bailey, Sabrina L.; Hambright, Peter
 CORPORATE SOURCE: Department of Chemistry, Howard University, Washington, DC, 20059, USA
 SOURCE: Inorganica Chimica Acta (2003), 344, 43-48
 CODEN: ICHAA3; ISSN: 0020-1693
 PUBLISHER: Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The kinetics of incorporation of Cu2+, Zn2+, Co2+, and Ni2+ into the free base H2-BrP(4)4+ and centrally monoprotoporphyrin H-BrP(4)3+ forms of the deformed and water soluble beta-octabromo-tetrakis(N-methyl-4-pyridyl)porphyrin were studied at 25 °C, I=0.10 (NaNO3/HNO3). Below pH 7, the reactions were first-order in porphyrin and metal, and the rate consts. increased with an increase in pH. The monocation H3-BrP(4)5+ did not incorporate metal ions, and H-BrP(4)3+ reacted several hundred times faster than H2-BrP(4)4+. The incorporation rate consts. for the pre-deformed H2-BrP(4)4+ were .apprx.103 times larger as compared to the more planar tetrakis(N-methyl-4-pyridyl)porphyrin. For both porphyrins, the reactivity order was Cu2+>Zn2+>Co2+>Ni2+. While Cu2+ reacted .apprx.104 times more rapidly than did Ni2+, the ratios of the metalation rate consts. of H-BrP(4)3+ to the water exchange rate consts. of the metal ions varied by no more than a factor of 4 across the series.
 IT 174580-25-7 503270-97-1
 RI: CYS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
 (kinetics of the reactions of divalent copper, zinc, cobalt, and nickel with a deformed water soluble centrally monoprotoporphyrin)
 RN 174580-25-7 CAPLUS
 CN Pyridinium, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis(1-methyl- (9CI) (CA INDEX NAME)



L6 ANSWER 22 OF 148 CAPLUS COPYRIGHT 2005 ACS ON STN (Continued)
 RN 503270-97-1 CAPLUS
 CN Pyridinium, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis(1-methyl-, mono(inner salt) (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

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REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2002:900049 CAPLUS

DOCUMENT NUMBER: 138:304092

TITLE: Photoinitiated olefin epoxidation with molecular oxygen, sensitized by free base porphyrins and promoted by hexacarbonylmolybdenum in homogeneous solution

AUTHOR(S): Campestri, Sandro; Tonellato, Umberto
CORPORATE SOURCE: Universita di Padova, Dipartimento di Chimica Organica, Centro CNR di Studio sui Meccanismi di Reazioni Organiche, Padova, 35131, Italy

SOURCE: European Journal of Organic Chemistry (2002), (22), 3827-3832
CODEN: EJOCFK; ISSN: 1434-193X

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:304092

AB The photooxidn. of various olefins in homogeneous solution under an oxygen atmosphere, by use of visible light, a dye sensitizer, and an oxygen-transfer

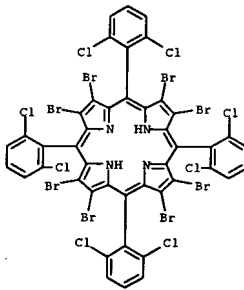
catalyst, has been investigated. The oxygen transfer from mol. oxygen to olefin involves the following steps: (i) photoinduced singlet-oxygen formation, (ii) alkyl hydroperoxide formation through the ene reaction, (iii) the intermediacy of a reactive molybdenum peroxide, and (iv) olefin epoxidn. of the remaining substrate or of a second olefin. Among the various sensitizers and catalysts tested, the electron-deficient free base porphyrin 5,10,15,20-tetrakis(2',6'-dichlorophenyl)-p-octabromoporphyrin and hexacarbonylmolybdenum showed the best performances in terms of robustness and activity. Under suitable conditions, complete olefin conversion can be obtained by adoption of molar ratios of sensitizer/catalyst/substrate of 1:50:2000, with the formation of the corresponding epoxide in up to 38% yield, which corresponds to 77% of the theor. maximum. Quite interestingly, olefins reluctant to undergo ene reactions may be epoxidized in the presence of a second sacrificial olefin, yielding the corresponding epoxides with up to 80% total selectivity.

IT 107035-95-0

RL: RGT (Reagent); RACT (Reactant or reagent)
(photoinitiated olefin epoxidn. with mol. oxygen sensitized by free base porphyrine and promoted by hexacarbonylmolybdenum)

RN 107035-95-0 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,6-dichlorophenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2002:808700 CAPLUS

DOCUMENT NUMBER: 138:73108

TITLE: On the role of β -fluorine substitution on the extent of core deformation of porphyrin dications

AUTHOR(S): Forhiel, Emmanuel; Toupet, Loic; Leroy, Jacques;
CORPORATE SOURCE: Bondon, Arnaud

SOURCE: Laboratoire de Chimie Organometallique et Biologique, Universite de Rennes 1, UMR CNRS 6509, Rennes, F-35042, Fr.

Tetrahedron Letters (2002), 43(46), 8293-8296

CODEN: TELEAY; ISSN: 0040-4039

Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Careful anal. of fully and partially β -fluorinated dicationic porphyrins have been performed suggesting an electronic influence of the β -fluorine atoms on the extent of the macrocycle deformation, in agreement with the crystal structure of β -octafluoro-meso-tetraphenylporphyrin dication.

IT 479637-18-8P

RL: FNU (Preparation, unclassified); PRP (Properties); PREP (Preparation)
(crystal structure; role of β -fluorine substitution on the extent of core deformation of porphyrin dications)

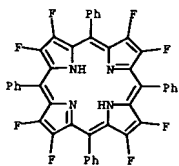
RN 479637-18-8 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetraphenyl-, diperchlorate, compd. with dichloromethane (1:2), dihydrate (9CI) (CA INDEX NAME)

CH 1

CRN 186885-28-9

CMF C44 H22 F8 N4



CH 2

CRN 7601-90-3

CMF C1 H 04



CH 3

CRN 75-09-2

CMF C H2 Cl2

Cl-CH2-Cl

IT 479637-13-3 479637-15-5

RL: PRP (Properties)
(role of β -fluorine substitution on the extent of core deformation of porphyrin dications)

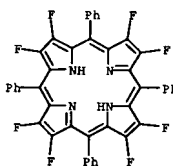
RN 479637-13-3 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetraphenyl-, diperchlorate (9CI) (CA INDEX NAME)

CH 1

CRN 186885-28-9

CMF C44 H22 F8 N4



CH 2

CRN 7601-90-3

CMF C1 H 04



RN 479637-15-5 CAPLUS

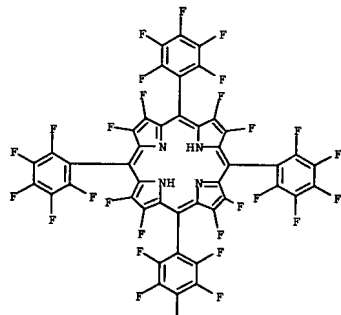
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)-, diperchlorate (9CI) (CA INDEX NAME)

CH 1

CRN 121399-88-0

CMF C44 H2 F28 N4

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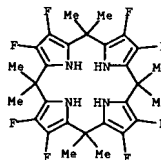
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CN 2

CRN 7601-90-3
CMF C1 H O4

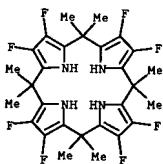
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 25 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2002:751572 CAPLUS
 DOCUMENT NUMBER: 137:389723
 TITLE: Theoretical Study of Anion Binding to Calix[4]pyrrole: the Effects of Solvent, Fluorine Substitution, Cosolute, and Water Traces
 AUTHOR(S): Blas, J. Ramon; Marquez, Manuel; Sessler, Jonathan L.; Luque, F. Javier; Orozco, Modesto
 CORPORATE SOURCE: Departament de Bioquímica i Biologia Molecular, Facultat de Química, Universitat de Barcelona, Barcelona, 08028, Spain
 SOURCE: Journal of the American Chemical Society (2002), 124(43), 12796-12805
 CODEN: JACSAT; ISSN: 0002-7863
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The binding of different anions to calix[4]pyrrole has been studied by means of mol. dynamics coupled to thermodyn. integration calcs. The effect of different apolar solvents, octafluoro substitution, and the change in binding free energy derived from the presence of cosolute and water traces (the hydrated salt used to introduce the anion in the solution) were examined. Calcs. allow us to rationalize the differential binding of ions to calix[4]pyrrole and octafluorocalix[4]pyrrole as well as to predict the behavior in new solvents for which exptl. data are not available yet. It is found that both calix[4]pyrrole and octafluorocalix[4]pyrrole have a dramatic preference for F⁻ in the gas phase and pure aprotic solvents, but the situation can change dramatically in protic solvents or in the presence of the hydrated cation which is used as cosolute of the anion. Overall, our results provide interesting clues for a better understanding of the process detected exptl. as "binding".
 IT 311804-81-6
 RL: PEP (Physical, engineering or chemical process); PRF (Properties); PYP (Physical process); PROC (Process)
 (effects of solvents and fluorine substitution on anion binding to calix[4]pyrrole from mol. dynamics and thermodyn. integration)
 RN 311804-81-6 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)



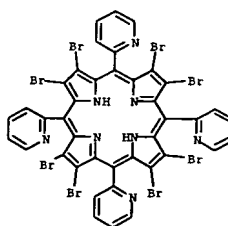
IT 475644-56-5
 RL: FMU (Formation, unclassified); PRF (Properties); FORM (Formation, nonpreparative)
 (optimized mol. structure of chloride-octafluorocalix[4]pyrrole, fluoride-calix[4]pyrrole, phosphate-calix[4]pyrrol, and fluoride-tetrabutylammonium trihydrate complexes)
 RN 475644-56-5 CAPLUS

L6 ANSWER 25 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
 CN Chloride, compd. with 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)

● Cl⁻

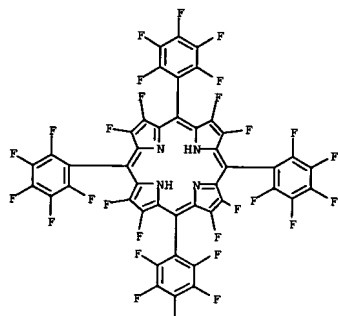
REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 26 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2002:749114 CAPLUS
 DOCUMENT NUMBER: 138:48962
 TITLE: Perhalogenated 2-pyridylporphyrin complexes: synthesis, self-coordinating aggregation properties, and catalytic studies
 AUTHOR(S): Reboucas, Julio S.; De Carvalho, Maria Eliza M. D.; Idemori, Ynara M.
 CORPORATE SOURCE: Departamento de Química - ICEX - Universidade Federal de Minas Gerais, Belo Horizonte, 31270-901, Brazil
 SOURCE: Journal of Porphyrins and Phthalocyanines (2002), 6(1), 50-57
 CODEN: JPPHFZ; ISSN: 1088-4246
 PUBLISHER: Society of Porphyrins & Phthalocyanines
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 138:48962
 AB The synthesis of 2,3,7,8,12,13,17,18-octabromo-meso-tetrakis(2-pyridyl)porphyrin, H2Br8T2PyP, is described, including the comparison of four attempted methods for the demetalation of ZnBr8T2PyP. One of the methods represents a strategy of demetalation based on the acid-base properties of the macrocycle, the solvent-dependent kinetics of metal insertion into porphyrins and the pH-dependent solubility of the 2-pyridylporphyrin derivs. in water. Self-coordinating aggregation of ZnBr8T2PyP in non-coordinating solvents was verified by 1H NMR spectroscopy. The Mn(III)/Mn(II) redox potential for MnBr8T2PyPCl is 0.38 V higher than the reduction potential measured for its 1st-generation analog, MnT2PyPCl. Cyclohexane hydroxylation by iodosylbenzene was performed in CH3CN catalyzed by MnBr8T2PyPCl and MnT2PyPCl. MnBr8T2PyPCl was highly active, even at low concentration (5 + 10⁻⁵ M), but perhalogenation did not account for oxidative robustness. At such a low catalyst concentration, MnT2PyPCl exhibited no activity as inferred by comparison to blank expts.
 IT 478363-47-2
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (reactant for preparation of manganese perhalogenated tetrakis(pyridyl)porphyrinato complexes)
 RN 478363-47-2 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetra-2-pyridinyl- (9CI) (CA INDEX NAME)



L6 ANSWER 27 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2002:725874 CAPLUS
 DOCUMENT NUMBER: 138:49060
 TITLE: Synthesis of F28 tetraphenylporphyrin and its application to the separation and detection of lithium (I)
 AUTHOR(S): Koyanagi, Kenji; Tabata, Masaaki
 CORPORATE SOURCE: Department of Chemistry, Faculty of Science and Engineering, Saga University, 1-Honjo-machi, Saga-shi, Saga, 840-8502, Japan
 SOURCE: Bunseki Kagaku (2002), 51(9), 803-807
 CODEN: BNSKAK; ISSN: 0525-1931
 PUBLISHER: Nippon Bunseki Kagakkai
 DOCUMENT TYPE: Journal
 LANGUAGE: Japanese
 AB 2,3,7,8,12,13,17,18-Octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)porphyrin (F28 tetraphenylporphyrin; OFTPFPF) was synthesized by the condensation of 3,4-difluoropyrrole and pentafluorobenzaldehyde. 3,4-Difluoropyrrole was prepared from 2,2,3,3-tetrafluorosuccinic acid as the starting material through 5-step reaction processes. The acid-dissociation consts. of OFTPFPF were determined by a solvent-extraction method in the presence of tetrabutylammonium chloride (0.1 mol dm⁻³). The 28 fluorine atoms decreased the basicity of the porphyrin and made two protons of imidazoles release at pH 4 and 7 ((H2P)⁰ + Na⁺ .dblfharw. [(HP⁻)(Na⁺)₂], pKa3 4.2; [(HP⁻)(Na⁺)₂]⁰ + Na⁺ .dblfharw. [(P2⁻)(Na⁺)₂]₂, pKa4 8.0). The protons of the tetraphenylporphyrin unsubstituted by fluorine atom did not dissociate at a pH lower than 14. OFTPFPF reacted with lithium ion in the neutral pH range, and gave a new absorption spectrum with a maximum wavelength of 416 nm in chloroform.
 IT 121399-88-0P
 RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis of F28 tetraphenylporphyrin and separation and detection of lithium)
 RN 121399-88-0 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

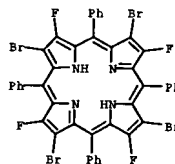
PAGE 1-A



PAGE 2-A

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F

L6 ANSWER 28 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2002:641275 CAPLUS
 DOCUMENT NUMBER: 137:379220
 TITLE: Synthesis and characterization of partially β -fluorinated 5,10,15,20-tetraphenylporphyrins and some derivatives
 AUTHOR(S): Leroy, Jacques; Porbiel, Emmanuel; Bondon, Arnaud
 CORPORATE SOURCE: UMR CNRS 8640, Departement de Chimie, Ecole Normale Supérieure, Paris, 75231, Fr.
 SOURCE: Tetrahedron (2002), 58(33), 6713-6722
 CODEN: TETRAH; ISSN: 0040-4020
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 137:379220
 AB The synthesis of partially β -fluorinated meso-tetraphenylporphyrins using Lindsey conditions, was examined, starting either from 3,4-difluoro-1H-pyrrole or from 3-fluoro-1H-pyrrole. In the case of the 1st synthon, condensation with pyrrole and benzaldehyde afforded a mixture of porphyrins of general formula β -FnTPP (n = 0,2,4,6,8) displaying linearly correlated spectroscopic and electrochem. properties. With the 2nd synthon, condensation with benzaldehyde produced an unresolvable mixture of β -tetrafluoroporphyrins presenting spectroscopic and electrochem. properties in coherence with those observed in the 1st case. Preliminarily, the synthesis and isolation of the hitherto unknown 3-fluoro-1H-pyrrole was approached via several methods. Preparation of zinc complexes of the fluorinated porphyrins is reported.
 IT 475561-96-7P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation of partially β -fluorinated porphyrins and their zinc complexes)
 RN 475561-96-7 CAPLUS
 CN 21H,23H-Porphine, 2,7,12,17-tetrabromo-3,8,13,18-tetrafluoro-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



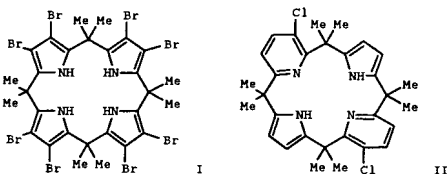
L6 ANSWER 29 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2002:638268 CAPLUS
 DOCUMENT NUMBER: 137:185360
 TITLE: Preparation, binding properties, and uses of halogenated calixpyrroles, calixpyridinopyrroles and calixpyridines
 INVENTOR(S): Sessler, Jonathan L.; Marquez, Manuel; Anzenbacher, Pavel; Shriver, James A.
 PATENT ASSIGNEE(S): USA
 SOURCE: U.S. Pat. Appl. Publ., 104 pp., Cont.-in-part of U.S. Ser. No. 838,998.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002115566	A1	20020822	US 2001-939514	20010824
CA 2391030	AA	19971016	CA 1997-2391030	19970404
US 6262257	B1	20010717	US 1997-833379	19970404
US 2002026047	A1	20020228	US 2001-838998	20010420
WO 2003018548	A2	20030306	WO 2002-US27252	20020826
WO 2003018548	A3	20030703		

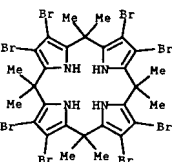
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 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:
 US 1996-14890P P 19960405
 US 1996-24203P P 19960827
 US 1996-26694P P 19960925
 US 1996-33395P P 19961217
 US 1996-33396P P 19961217
 US 1997-833379 A3 19970404
 US 2001-838998 A2 20010420
 CA 1997-2251072 A3 19970404
 US 2001-939514 A 20010824

OTHER SOURCE(S):
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L6 ANSWER 29 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

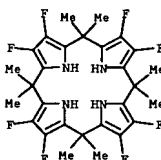


L6 ANSWER 29 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

AB Halogenated calixpyrrole, calixpyridinopyrrole, and calixpyridine macrocycles, such as octabromo-meso-octamethylcalix[4]pyrrole (I) and calixpyridinopyrrole II, having 4-12 pyrrolic rings with greater stability were prepared for uses such as dialysis, ion exchange, and environmental remediation. Thus, I was prepared in 90% yield by bromination of the corresponding meso-octamethylcalix[4]pyrrole using N-bromosuccinimide in THF. Enhanced anion, neutral mol. binding affinity and different binding selectivities as compared to their nonhalogenated congeners as judged from ¹H NMR, ¹⁹F NMR and fluorescence emission spectroscopic analyses.

IT 311804-81-6P
 RL: NUU (Other use, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PTP (Physical process); SPW (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
 (preparation and anion binding properties of calixpyrroles, calixpyridinopyrroles and calixpyridines for use environmental remediation, kidney dialysis and cation exchangers)

RN 311804-81-6 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)



IT 190517-33-0P
 RL: NUU (Other use, unclassified); PEP (Physical, engineering or chemical process); PTP (Physical process); SPW (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
 (preparation and anion binding properties of calixpyrroles, calixpyridinopyrroles and calixpyridines for use environmental remediation, kidney dialysis and cation exchangers)

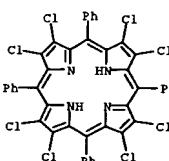
RN 190517-33-0 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)

L6 ANSWER 30 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2002:626618 CAPLUS
 DOCUMENT NUMBER: 139:197287
 TITLE: Lewis-base binding properties of free-base β-octahalotetraphenylporphyrins. [Erratum to document cited in CA137:279005]
 AUTHOR(S): Bhyrappa, P.; Bhavana, P.
 CORPORATE SOURCE: Department of Chemistry, Indian Institute of Technology, Chennai, 600 036, India
 SOURCE: Chemical Physics Letters (2002), 360(5,6), 592
 CODEN: CHPLBC; ISSN: 0009-2614
 PUBLISHER: Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

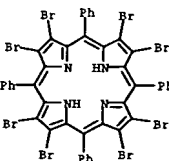
AB In the Abstract, line 2, "The kinetics of base..." should be "The base...". On page 108, paragraph 3, line 9, "The kinetics of anion..." should be "The anion...". On page 109, paragraph 1, lines 4 and 5, "nitrogenous bases, kinetics of base..." should be "nitrogenous bases, base...".

IT 120644-25-9, 2,3,7,8,12,13,17,18-Octachloro-5,10,15,20-tetraphenylporphyrin 131214-86-3, 2,3,7,8,12,13,17,18-Octabromo-5,10,15,20-tetraphenylporphyrin
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
 (binding with Lewis acid bases; Lewis-base binding properties of free-base β-octahalotetraphenylporphyrins (Erratum))

RN 120644-25-9 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



RN 131214-86-3 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



IT 465536-78-1P 465536-80-5P 465536-81-6P
 465536-84-9P 465536-87-2P 465536-90-7P
 465536-91-8P 465536-92-9P 465536-93-0P
 465536-95-2P 465536-96-3P 465536-97-4P
 465536-98-5P 465536-99-6P 465537-00-2P
 465537-01-3P

RI: CPS (Chemical process); PEP (Physical, engineering or chemical process); FRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
 (preparation of, formation const. for; Lewis-base binding properties of free-base β -octahalotetraphenylporphyrins (Erratum))

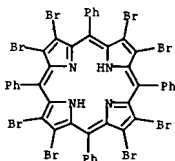
RN 465536-78-1 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-, compd. with quinoline (1:1) (9CI) (CA INDEX NAME)

CH 1

CRN 131214-86-3

CMF C44 H22 Br8 N4



CH 2

CRN 91-22-5

CMF C9 H7 N



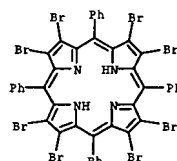
RN 465536-80-5 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-, compd. with pyridine (1:1) (9CI) (CA INDEX NAME)

CH 1

CRN 131214-86-3

CMF C44 H22 Br8 N4



CH 2

CRN 110-86-1

CMF C5 H5 N



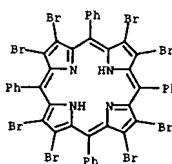
RN 465536-81-6 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-, compd. with 3-methylpyridine (1:1) (9CI) (CA INDEX NAME)

CH 1

CRN 131214-86-3

CMF C44 H22 Br8 N4



CH 2

CRN 108-99-6

CMF C6 H7 N



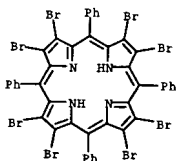
RN 465536-84-9 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-, compd. with 1-methyl-1H-imidazole (1:1) (9CI) (CA INDEX NAME)

CH 1

CRN 131214-86-3

CMF C44 H22 Br8 N4



CH 2

CRN 616-47-7

CMF C4 H6 N2



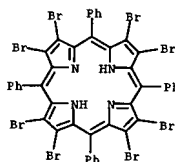
RN 465536-87-2 CAPLUS

CN 4-Pyridinamine, N,N-dimethyl-, compd. with 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)

CH 1

CRN 131214-86-3

CMF C44 H22 Br8 N4



CH 2

CRN 1122-58-3

CMF C7 H10 N2



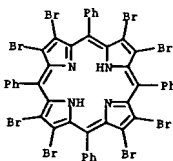
RN 465536-90-7 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-, compd. with piperidine (1:1) (9CI) (CA INDEX NAME)

CH 1

CRN 131214-86-3

CMF C44 H22 Br8 N4



CH 2

CRN 110-89-4

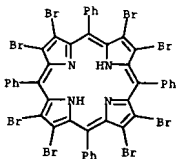
CMF C5 H11 N



RN 465536-91-8 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-,
compd. with 1,4-dioxane (1:1) (9CI) (CA INDEX NAME)

CH 1

CRN 131214-86-3
CMF C44 H22 Br8 N4



CH 2

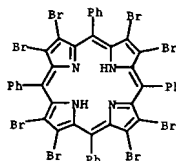
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CMF C4 H8 O2



RN 465536-92-9 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-,
compd. with sulfinylbis[methane] (1:1) (9CI) (CA INDEX NAME)

CH 1

CRN 131214-86-3
CMF C44 H22 Br8 N4



CH 2

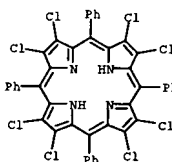
CRN 67-68-5
CMF C2 H6 O S



RN 465536-93-0 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-,
compd. with quinoline (1:1) (9CI) (CA INDEX NAME)

CH 1

CRN 120644-25-9
CMF C44 H22 Cl8 N4



CH 2

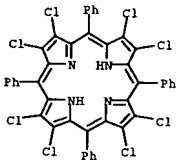
CRN 91-22-5
CMF C9 H7 N



RN 465536-95-2 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-,
compd. with pyridine (1:1) (9CI) (CA INDEX NAME)

CH 1

CRN 120644-25-9
CMF C44 H22 Cl8 N4



CH 2

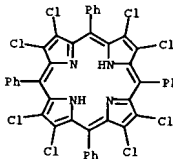
CRN 110-86-1
CMF C5 H5 N



RN 465536-96-3 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-,
compd. with 3-methylpyridine (1:1) (9CI) (CA INDEX NAME)

CH 1

CRN 120644-25-9
CMF C44 H22 Cl8 N4



CH 2

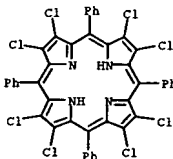
CRN 108-99-6
CMF C6 H7 N



RN 465536-97-4 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-,
compd. with 1-methyl-1H-imidazole (1:1) (9CI) (CA INDEX NAME)

CH 1

CRN 120644-25-9
CMF C44 H22 Cl8 N4



CH 2

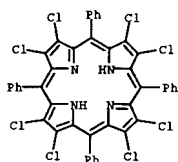
CRN 616-47-7
CMF C4 H6 N2



RN 465536-98-5 CAPLUS
CN 4-Pyridinamine, N,N-dimethyl-, compd. with 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 120644-25-9
CMF C44 H22 C18 N4



CM 2

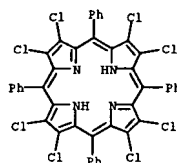
CRN 1122-58-3
CMF C7 H10 N2



RN 465536-99-6 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-, compd. with piperidine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 120644-25-9
CMF C44 H22 C18 N4



CM 2

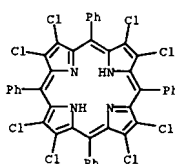
CRN 110-89-4
CMF C5 H11 N



RN 465537-00-2 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-, compd. with 1,4-dioxane (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 120644-25-9
CMF C44 H22 C18 N4



CM 2

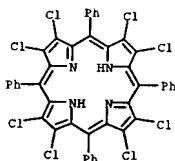
CRN 123-91-1
CMF C4 H8 O2



RN 465537-01-3 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-, compd. with sulfinylbis[methane] (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 120644-25-9
CMF C44 H22 C18 N4

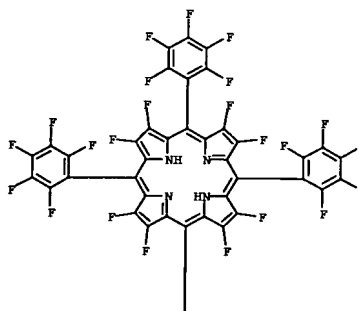


CM 2

CRN 67-68-5
CMF C2 H6 O S



ACCESSION NUMBER: 2002:626587 CAPLUS
DOCUMENT NUMBER: 137:352662
TITLE: Theoretical studies on the structural change of the N-protonated tetraphenylporphyrin. (II) - effects of the substituting fluorine groups
AUTHOR(S): Huang, Xiao-Fen; Ma, Si-Yu; Liu, Ruo-Zhuang
CORPORATE SOURCE: Department of Chemistry, Beijing Normal University, Beijing, 100875, Peop. Rep. China
SOURCE: Gaodeng Xuexiao Huaxue Xuebao (2002), 23(8), 1562-1566
CODEN: KTHFDM; ISSN: 0251-0790
PUBLISHER: Gaodeng Jiaoyu Chubanshe
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB With the symmetry being reasonably restricted, the semi-empirical method of AM1 MO is used to calculate the geometries of 5,10,15,20-tetrakis(pentafluorophenyl)porphyrin (TF5PPH2) and 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)porphyrin (F28TPPH2) and their N-protonated diacids (TF5PPH2+4 and F28TPPH2+4) which all are kinds of important porphyrin derivs. Also, the configurational change in protonation process and the probable influence to mol. aggregation conducted by the change are discussed by the means of structure anal., population anal. and frontier orbital anal.
IT 474422-37-2
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(theor. studies on fluorine substituent effects on structural changes by N-protonation of tetraphenylporphyrin)
RN 474422-37-2 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)-, conjugate diacid (9CI) (CA INDEX NAME)



PAGE 2-A

● 2 H⁺

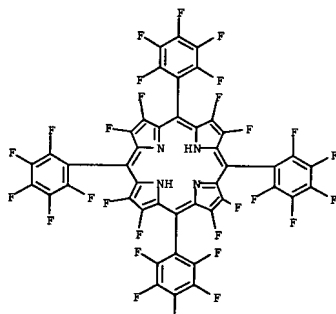
IT 121399-88-0

RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(theor. studies on fluorine substituent effects on structural changes
by N-protonation of tetraphenylporphyrin)

RN 121399-88-0 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-
tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

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F

PAGE 2-A

ACCESSION NUMBER: 2002:624523 CAPLUS

DOCUMENT NUMBER: 139:220923

TITLE: Unusual solvent dependent optical absorption spectral
properties of free base perhaloporphyrins. [Erratum to
document cited in CA135:263667]

AUTHOR(S): Bhyrappa, P.; Bhavana, P.
CORPORATE SOURCE: Department of Chemistry, Indian Institute of
Technology, Madras, Chennai, 600 036, India
SOURCE: Chemical Physics Letters (2002), 360(5,6), 592
CODEN: CHPLBC; ISSN: 0009-2614
PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal
LANGUAGE: English

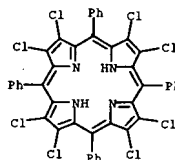
AB In Table 3, last data line, H2OSTPP should be H2TTP. On page 43,
paragraph 4, line 2, 1.70 should be -1.70; in line 3, 0.1 should be -0.10.

IT 120644-25-9, 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-
5,10,15,20-tetraphenyl- 131214-86-3, 2,3,7,8,12,13,17,18-
Octabromo-5,10,15,20-tetraphenylporphyrin

RL: PRP (Properties)
(unusual solvent dependent optical absorption spectral properties of
free-base perhaloporphyrins (Erratum))

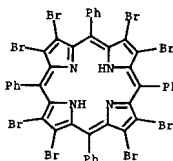
RN 120644-25-9 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-
(9CI) (CA INDEX NAME)



RN 131214-86-3 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-
(9CI) (CA INDEX NAME)



ACCESSION NUMBER: 2002:424652 CAPLUS

DOCUMENT NUMBER: 137:155101

AUTHOR(S): Catalytic Oxidations of Steroid Substrates by
Artificial Cytochrome P-450 Enzymes
Yang, Jerry; Gabriele, Bartolo; Belvedere, Sandro;
Huang, Ying; Breslow, Ronald

CORPORATE SOURCE: Department of Chemistry, Columbia University, New
York, NY, 10027, USA

SOURCE: Journal of Organic Chemistry (2002), 67(15), 5057-5067
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:155101

AB Catalysts comprising manganese-porphyrins carrying cyclodextrin binding
groups are able to perform hydroxylations with substrate selectivity and
regio- and stereoselectivity and high catalytic turnovers. The geometries
of the catalyst/substrate complexes override intrinsic substrate
reactivities, permitting attack on geometrically accessible saturated

carbons of steroids in the presence of secondary carbinol groups and carbon-carbon
double bonds, as in enzymic reactions. Selective hydroxylations of
steroid carbon 9 positions are of particular practical interest.

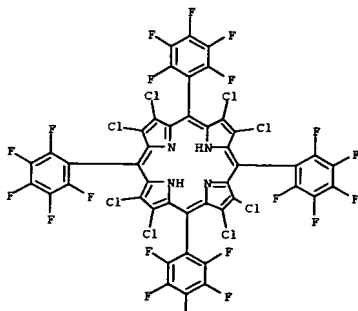
IT 161405-60-3P, 2,3,7,8,12,13,17,18-Octachloro-5,10,15,20-Tetrakis(4-
mercapto-2,3,5,6-tetrafluorophenyl)porphyrin

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(regio- and stereoselective catalytic oxidns. of steroids by catalysts
comprising manganese-porphyrins bound to cyclodextrins)

RN 161405-60-3 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-
tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

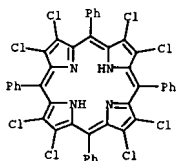
|
F

REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 34 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2002:338995 CAPLUS
 DOCUMENT NUMBER: 137:279005
 TITLE: Lewis-base binding properties of free-base
 8-octahalotetraphenylporphyrins
 AUTHOR(S): Bhayappa, P.; Bhavana, P.
 CORPORATE SOURCE: Department of Chemistry, Indian Institute of
 Technology, Chennai, 600 036, India
 SOURCE: Chemical Physics Letters (2002), 357(1,2), 108-112
 CODEN: CHPLBC; ISSN: 0009-2614
 PUBLISHER: Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

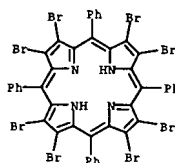
AB Sym. substituted perhaloporphyrins, 2,3,7,8,12,13,17,18-octahalo (bromo
 and chloro)-5,10,15,20-tetraphenylporphyrins (H2OBTPP and H2OCTPP) have
 been examined as receptors for binding to Lewis bases. The kinetics of base
 binding to haloporphyrins showed an enhanced binding consts. for H2OBTPP
 relative to H2OCTPP and follows a linear trend with increase in pKa values
 of the bases. The binding of Lewis-bases to perhaloporphyrin core is
 largely influenced by the extent of nonplanarity of the porphyrin core
 than the electron-withdrawing ability of the substituents. The higher
 binding consts. of H2OBTPP relative to H2OCTPP have been interpreted in
 terms of greater nonplanarity of the former than the latter.

IT 120644-25-9, 2,3,7,8,12,13,17,18-Octachloro-5,10,15,20-
 tetraphenylporphyrin 131214-86-3, 2,3,7,8,12,13,17,18-Octabromo-
 5,10,15,20-tetraphenylporphyrin
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical
 process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
 (binding with Lewis acid bases; Lewis-base binding properties of
 free-base 8-octahalotetraphenylporphyrins)
 RN 120644-25-9 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-
 (9CI) (CA INDEX NAME)



RN 131214-86-3 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-
 (9CI) (CA INDEX NAME)

L6 ANSWER 34 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

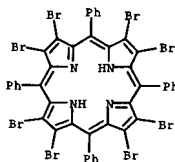


IT 465536-78-1P 465536-80-5P 465536-81-6P
 465536-84-9P 465536-87-2P 465536-90-7P
 465536-91-8P 465536-92-9P 465536-93-0P
 465536-95-2P 465536-96-3P 465536-97-4P
 465536-98-5P 465536-99-6P 465537-00-2P
 465537-01-3P

RL: CPS (Chemical process); PEP (Physical, engineering or chemical
 process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
 (preparation of, formation consts. for; Lewis-base binding properties of
 free-base 8-octahalotetraphenylporphyrins)

RN 465536-78-1 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-,
 compd. with quinoline (1:1) (9CI) (CA INDEX NAME)

CM 1
 CRN 131214-86-3
 CMF C44 H22 Br8 N4



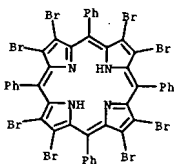
CM 2
 CRN 91-22-5
 CMF C9 H7 N



L6 ANSWER 34 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 465536-80-5 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-,
 compd. with pyridine (1:1) (9CI) (CA INDEX NAME)

CM 1
 CRN 131214-86-3
 CMF C44 H22 Br8 N4

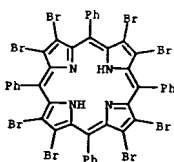


CM 2
 CRN 110-86-1
 CMF C5 H5 N



RN 465536-81-6 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-,
 compd. with 3-methylpyridine (1:1) (9CI) (CA INDEX NAME)

CM 1
 CRN 131214-86-3
 CMF C44 H22 Br8 N4



CM 2

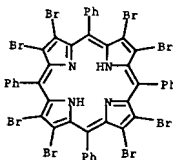
L6 ANSWER 34 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

CRN 108-99-6
 CMF C6 H7 N



RN 465536-84-9 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-,
 compd. with 1-methyl-1H-imidazole (1:1) (9CI) (CA INDEX NAME)

CM 1
 CRN 131214-86-3
 CMF C44 H22 Br8 N4

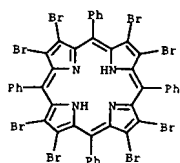


CM 2
 CRN 616-47-7
 CMF C4 H6 N2



RN 465536-87-2 CAPLUS
 CN 4-Pyridinamine, N,N-dimethyl-, compd. with 2,3,7,8,12,13,17,18-octabromo-
 5,10,15,20-tetraphenyl-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)

CM 1
 CRN 131214-86-3
 CMF C44 H22 Br8 N4

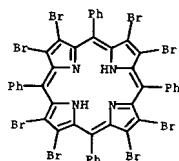


CM 2

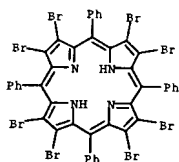
CRN 1122-58-3
CMF C7 H10 N2

RN 465536-90-7 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-,
compd. with piperidine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 131214-86-3
CMF C44 H22 Br8 N4

CM 2

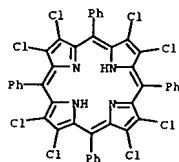
CRN 110-89-4
CMF C5 H11 N

CM 2

CRN 67-68-5
CMF C2 H6 O S

RN 465536-93-0 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-,
compd. with quinoline (1:1) (9CI) (CA INDEX NAME)

CM 1

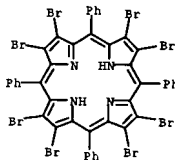
CRN 120644-25-9
CMF C44 H22 Cl8 N4

CM 2

CRN 91-22-5
CMF C9 H7 N

RN 465536-91-8 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-,
compd. with 1,4-dioxane (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 131214-86-3
CMF C44 H22 Br8 N4

CM 2

CRN 123-91-1
CMF C4 H8 O2

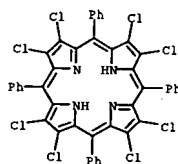
RN 465536-92-9 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-,
compd. with sulfinylbis[methane] (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 131214-86-3
CMF C44 H22 Br8 N4

RN 465536-95-2 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-,
compd. with pyridine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 120644-25-9
CMF C44 H22 Cl8 N4

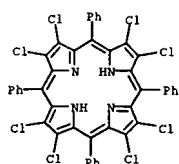
CM 2

CRN 110-86-1
CMF C5 H5 N

RN 465536-96-3 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-,
compd. with 3-methylpyridine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 120644-25-9
CMF C44 H22 Cl8 N4

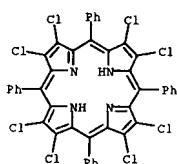


CM 2

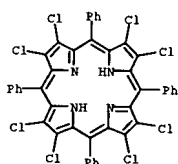
CRN 108-99-6
CMF C6 H7 N

RN 465536-97-4 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-,
compd. with 1-methyl-1H-imidazole (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 120644-25-9
CMF C44 H22 C18 N4

CM 2

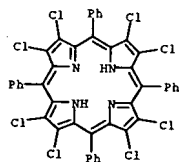
CRN 616-47-7
CMF C4 H6 N2

CM 2

CRN 110-89-4
CMF C5 H11 N

RN 465537-00-2 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-,
compd. with 1,4-dioxane (1:1) (9CI) (CA INDEX NAME)

CM 1

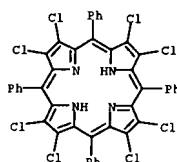
CRN 120644-25-9
CMF C44 H22 C18 N4

CM 2

CRN 123-91-1
CMF C4 H8 O2

RN 465536-98-5 CAPLUS
CN 4-Pyridinamine, N,N-dimethyl-, compd. with 2,3,7,8,12,13,17,18-octachloro-
5,10,15,20-tetraphenyl-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 120644-25-9
CMF C44 H22 C18 N4

CM 2

CRN 1122-58-3
CMF C7 H10 N2

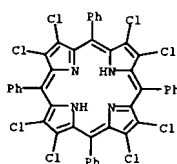
RN 465536-99-6 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-,
compd. with piperidine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 120644-25-9
CMF C44 H22 C18 N4

RN 465537-01-3 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-,
compd. with sulfanylbis[methane] (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 120644-25-9
CMF C44 H22 C18 N4

CM 2

CRN 67-68-5
CMF C2 H6 O S

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2002:337886 CAPLUS
DOCUMENT NUMBER: 137:194452

TITLE: Immobilization of β halogenated ironporphyrin in the silica matrix by the sol-gel process
AUTHOR(S): Aparecida Vidoto, Ednalvar Silva Monsalves Moreira, Maria da Silva Vinhado, Fabio Cluffi, Katia Jorge, Rangel Nascimento, Otaciro Yamamoto, Yassuko
CORPORATE SOURCE: Departamento de Quimica, Universidade de Sao Paulo, FFCLRP, Ribeirao Preto, SP, 14040-901, Brazil
SOURCE: Journal of Non-Crystalline Solids (2002), 304(1-3), 151-159
CODEN: JNCSEJ; ISSN: 0022-3093

PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The authors present the synthesis and characterization of a hybrid organic-inorg. material using robust metalloporphyrins halogenated in both meso and β -position, the iron complexes of 5,10,15,20-tetrakis(pentafluorophenyl)porphyrin and 2,3,7,8,12,13,17,18-octa- β -bromo-5,10,15,20-tetrakis(pentafluorophenyl)porphyrin, which stabilize the porphyrins against oxidative degradation. The immobilization was developed by the sol-gel process using pyridine and imidazole as template. EPR spectra of the iron complex of 2,3,7,8,12,13,17,18-octa- β -bromo-5,10,15,20-tetrakis(pentafluorophenyl)porphyrin show that the entrapment of ironporphyrin is in a higher symmetry compared to the systems in solution. A reduction of iron was observed in the presence of imidazole, determined by the absence of an EPR spectrum. The addition of chlorhydric acid vapor induced an oxidation of iron and a small quantity of iron in a high spin state was detected by a component with axial symmetry. The ironporphyrins were active as catalysts for cyclooctene epoxidn. using iodosylbenzene and hydrogen peroxide as oxygen donors. The perhalogenated porphyrins immobilized had a smaller activity due to their iron oxidation and spin states.

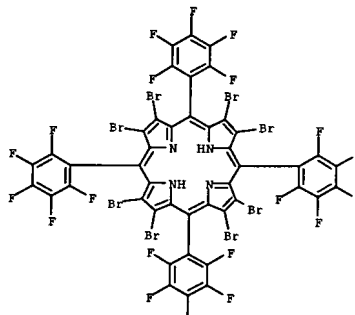
IT 139944-26-6P, 2,3,7,8,12,13,17,18-Octabromo-5,10,15,20-tetrakis(pentafluorophenyl)porphyrin
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(Intermediate; preparation of hybrid organic-inorg. materials of iron metalloporphyrins halogenated in meso and β -positions immobilized in silica matrix by sol-gel process)

RN 139944-26-6 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

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REFERENCE COUNT: 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2002:308212 CAPLUS
DOCUMENT NUMBER: 137:40848

TITLE: Comparative Study of Structure-Properties Relationship for Novel β -Halogenated Lanthanide Porphyrins and Their Nickel and Free Bases Precursors, as a Function of Number and Nature of Halogens Atoms
AUTHOR(S): Spyroulias, G. A.; Despotopoulos, A. P.; Raptopoulou, C. P.; Terzis, A.; de Montauzon, D.; Poilblanc, R.; Coutsolelos, A. G.
CORPORATE SOURCE: Department of Chemistry Laboratory of Bioinorganic Coordination Chemistry School of Science, University of Crete, Iraklion, Crete, 714 09, Greece
SOURCE: Inorganic Chemistry (2002), 41(10), 2648-2659
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:40848

AB The synthetic route of partially β -halogenated via a metal-assisted reaction and perhalogenated Tb complexes is described. This protocol allows the facile insertion of the halogens (bromines or chlorides) to the porphyrin peripheral positions. The electronic absorption spectra and the redox potentials of the free porphyrins as well as the Tb complexes are dramatically affected as the number of halogen atoms increases. In fact, two antagonistic effects are responsible for that, the inductive and the distortion effects on the porphyrin ring. They result in a red shift for the Soret band and a stabilization/destabilization of the HOMOs/LUMOs which in turn is manifested by variations on the redox potentials. The novel crystal structure of the Ni(Cl8TPP) is discussed in great detail and compared with the previously reported structures of Tb(Cl8TPP) (OAc) (DMF) 2-3PhCH₃-MeOH and H₂(Br8TPP), as well as with other perhalogenated Ni porphyrins available in the literature.

IT 189874-66-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal structure)

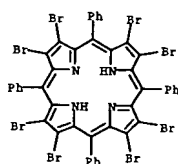
RN 189874-66-6 CAPLUS

CN Formamide, N,N-dimethyl-, compd. with 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-21H,23H-porphine (2:1) (9CI) (CA INDEX NAME)

CH 1

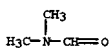
CRN 131214-86-3

CMF C44 H22 Br8 N4



CH 2

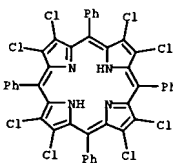
CRN 68-12-2
CMF C3 H7 N O



IT 120644-25-9P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation, electronic spectra, redox potentials and complexation with terbium(III))

RN 120644-25-9 CAPLUS

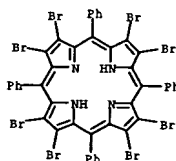
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



IT 131214-86-3P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation, mol. structure, electronic spectra, redox potentials and complexation with terbium(III))

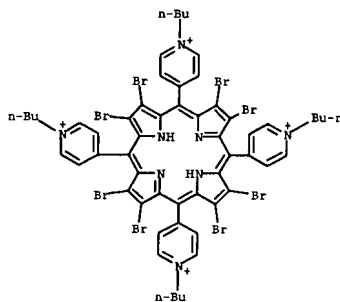
RN 131214-86-3 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 88 THERE ARE 88 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2002:218837 CAPLUS
 DOCUMENT NUMBER: 137:5840
 TITLE: Catalytic activity of tetraarylporphyrins in the oxidation reactions of saturated hydrocarbons
 AUTHOR(S): Avdeev, M. V.; Bagrii, E. I.; Maravin, G. B.; Korolev, Yu. M.
 CORPORATE SOURCE: Topchiev Institute of Petrochemical Synthesis, Russian Academy of Sciences, Moscow, 117912, Russia
 SOURCE: Kinetics and Catalysis (Translation of Kinetika i Kataliz) (2002), 43(1), 38-44
 CODEN: KICAA8; ISSN: 0023-1584
 PUBLISHER: MAIK Nauka/Interperiodica Publishing
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 137:5840
 AB Conference proceedings. The oxidation of cyclic hydrocarbons by potassium peroxymonosulfate catalyzed by the iron and manganese complexes of tetra-(4-N-butylpyridinium)porphyrin, tetraphenylporphyrin, and mixed porphyrins containing Ph and butylpyridyl substituents was studied in an aqueous acetonitrile medium. The test catalysts were dissolved in the reaction medium or adsorbed on layered aluminosilicates. It was found that the immobilization of metal complexes on layered aluminosilicates, as well as the bromination of porphyrins, decreased the activity of catalysts in a number of cases, although it improved their stability. The addition of pyridine in an equimolar amount with respect to metal complexes to the reaction mixture increased the activity of dissolved manganese complexes. An increase in the number of butylpyridyl meso-substituents in a porphyrin mol. improved the catalytic activity of a metal complex.
 IT 432028-75-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (Catalytic activity of tetraarylporphyrins in the oxidation reactions of saturated hydrocarbons)
 RN 432028-75-6 CAPLUS
 CN Pyridinium, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis[1-butyl-, tetraperchlorate (9CI) (CA INDEX NAME)
 CM 1
 CRN 432028-74-5
 CMF C56 H54 Br8 N8



CM 2

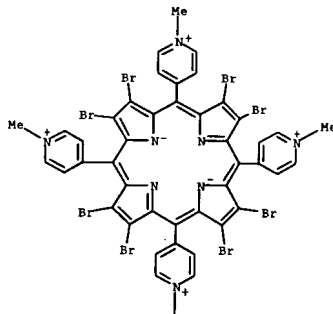
CRN 14797-73-0

CMF C1 O4



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2002:102683 CAPLUS
 DOCUMENT NUMBER: 136:331159
 TITLE: Kinetics of zinc ion incorporation in base into a centrally aprotic beta-octabrominated cationic water-soluble porphyrin and its monolithium complex
 AUTHOR(S): Bailey, Sabrina L.; Hambricht, P.
 CORPORATE SOURCE: Department of Chemistry, Howard University, Washington, DC, 20059, USA
 SOURCE: Journal of Porphyrins and Phthalocyanines (2001), 5(12), 829-834
 CODEN: JPPHFZ; ISSN: 1088-4246
 PUBLISHER: John Wiley & Sons Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The kinetics of zinc incorporation from pH 12 to 13 into the centrally aprotic BrP(4)2+ form of beta-octabromo-meso-tetrakis(N-methyl-4-pyridyl)porphyrin and its monolithium complex were studied at 25.0°C, ionic strength (I) = 0.10. The reactions were first order in porphyrin and total zinc concns. For BrP(4)2+, the specific rate constant was 5.1 x 105 M-1 s-1 for Zn(OH)2 aqueous 9.9 x 104 M-1 s-1 for Zn(OH)3-, and Zn(OH)42- was unreactive. The Li-BrP(4)3+ complex had a formation constant with BrP(4)2+ of 1.1 x 103 M-1 from both kinetic and equilibrium measurements. In solns. containing both BrP(4)2+ and Li-BrP(4)3+, zinc incorporation proceeded only through BrP(4)2+.
 IT 413578-85-5
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
 (kinetics of zinc ion incorporation in base into a centrally aprotic beta-octabrominated cationic water-soluble porphyrin and its monolithium complex)
 RN 413578-85-5 CAPLUS
 CN Pyridinium, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis[1-methyl-, bis(inner salt) (9CI) (CA INDEX NAME)



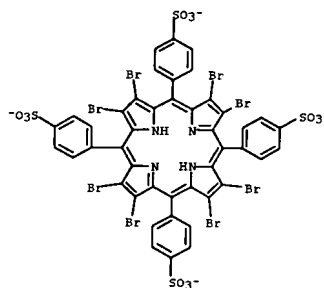
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REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 39 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:886633 CAPLUS
DOCUMENT NUMBER: 136:578
TITLE: Lithium detection in liquid biological samples and reagents therefor
INVENTOR(S): Balaze, Nicholas Dennis Henry; Secombe, John William
PATENT ASSIGNEE(S): Seba Diagnostics Pty. Ltd., Australia
SOURCE: PCT Int. Appl., 41 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

L6 ANSWER 39 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001092881	A1	20011206	WO 2001-AU603	20010525
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TH, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TH			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, MI, MR, NE, SN, TD, TG			
CA 2409971	AA	20011206	CA 2001-2409971	20010525
EP 1283986	A1	20030219	EP 2001-933464	20010525
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
US 2003186450	A1	20031002	US 2003-296592	20030604
PRIORITY APPL. INFO.:			AU 2000-7768	A 20000526
			WO 2001-AU603	W 20010525

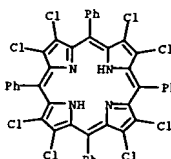
AB A method of detecting soluble lithium in a liquid biol. sample comprising combining: (a) an amount of the biol. sample; (b) 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(4-sulfonatophenyl) porphyrin; (c) alkali; (d) detergent; (e) chelating agent; and (f) optionally a suitable solvent; to produce a test sample; detecting absorbance change of the test sample relative to a lithium deficient standard sample at a wavelength of between about 475nm and about 485nm, between about 515nm and about 525nm or simultaneously between about 475nm and about 485nm and between about 515nm and about 525nm, wherein absorbance change indicates presence of soluble lithium in the biol. sample. Also disclosed is a method of quant. measuring soluble lithium ions in a biol. sample and a reagent for use in such methods.

IT 176173-80-1
RL: ANT (Analyte); ANST (Analytical study)
(lithium detection in liquid biol. samples and reagents therefor)
RN 176173-80-1 CAPLUS
CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis-, ion(4-) (9CI) (CA INDEX NAME)

L6 ANSWER 41 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:536788 CAPLUS
DOCUMENT NUMBER: 136:74895
TITLE: Conformational analysis of octa- and tetrahalogenated tetraphenylporphyrins and their metal derivatives
AUTHOR(S): Gruden, M.; Grubisic, S.; Coutsolelos, A. G.; Niketic, S. R.
CORPORATE SOURCE: Department of Chemistry, Faculty of Science, University of Belgrade, Belgrade, YU-11001, Yugoslavia
SOURCE: Journal of Molecular Structure (2001), 595(1-3), 209-224
CODEN: JMOSB4; ISSN: 0022-2860
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A new maximally diagonal force field for mol. modeling of metalloporphyrins is developed and optimized on the crystal structures of nickel(II) porphine, nickel(II) mono-tert-butylporphyrin and nickel(II) di-tert-butylporphyrin. It is then used to investigate non-planar distortions of octa- and tetrachloro tetraphenylporphyrins (TPP) and their Ni(II) and Tb(III) complexes. Mol. mechanics (MM) calcns. reproduced very well the structure of Tb(III) octachloro-TPP (so far the only example of a crystallog. characterized chloro TPP metal derivative). Normal-coordinate structural decomposition (NSD) anal. was performed on the equilibrium structures obtained by MM calcns. As expected, sad distortion dominates in octachloro structures irrespect of the presence or the size of the central metal atom; dom distortion dominates in tetrachloro structures with large Tb(III) central atom, while sad, ruf, wav and pro distortions are present in various amts. in other tetrachloro structures (TPP free base and Ni(II) complex) depending on the pattern of peripheral chloro substitution on the pyrrole rings. Other observed regularities are: reduction of the conformational flexibility of the porphyrin core upon metalation, and increase of the dihedral angle between the Ph groups and the mean LSQ plane of the porphyrin core, as well as the overall increase in structural regularity upon the increase of the size of the central metal atom.

IT 120644-25-9
RL: PRP (Properties)
(conformational anal. of octa- and tetrahalogenated tetraphenylporphyrins and metal derivs. with new maximally diagonal force field)
RN 120644-25-9 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

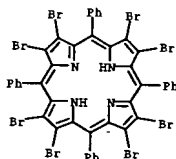


REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 40 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:732629 CAPLUS
DOCUMENT NUMBER: 136:37433
TITLE: Structure and physicochemical properties of substituted porphyrins
AUTHOR(S): Karmanova, T. V.; Gromova, T. V.; Berezin, B. D.; Semelkin, A. S.; Syrbu, S. A.
CORPORATE SOURCE: Ivanovo State University of Chemical Engineering, Ivanovo, Russia
SOURCE: Russian Journal of General Chemistry (Translation of Zhurnal Obshchei Khimii) (2001), 71(5), 803-808
CODEN: RUGCEK; ISSN: 1070-3632
PUBLISHER: MAIK Nauka/Interperiodica Publishing
DOCUMENT TYPE: Journal
LANGUAGE: English

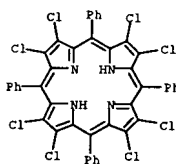
AB Reactions of substituted porphyrins: 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenylporphine, 2,3,7,8,12,13,17,18-octamethyl-5,10,15,20-tetraphenylporphine, and dodecaphenylporphine with organic bases (pyridine, piperidine, DMF, DMSO) and acetic acid were studied by spectrophotometry. Acid-base interaction between porphyrins and organic bases and formation of ionic species in toluene solution containing an organic base were revealed for the first time. The effect of electronic and structural factors on the acid-base interactions of porphyrin ligands with organic bases is discussed. The stability consts. were calculated for complexes of 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenylporphine with organic bases, and electronic absorption spectra of substituted porphyrins in basic organic solvents were recorded.

IT 131214-86-3
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(structure and physicochem. properties of substituted porphyrins)
RN 131214-86-3 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

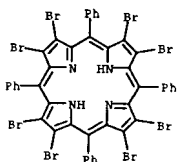


REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 42 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:488195 CAPLUS
DOCUMENT NUMBER: 135:263667
TITLE: Unusual solvent dependent optical absorption spectral properties of free-base perhaloporphyrins
AUTHOR(S): Bhyrappa, P.; Bhavana, P.
CORPORATE SOURCE: Department of Chemistry, Indian Institute of Technology, Madras, Chennai, 600 036, India
SOURCE: Chemical Physics Letters (2001), 342(1,2), 39-44
CODEN: CHPLBC; ISSN: 0009-2614
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A pair of free-base perhaloporphyrins, 2,3,7,8,12,13,17,18-octabromo- and octachloro-5,10,15,20-tetraphenylporphyrins (H2OBTTP and H2OCTTP) were examined in solvents of varying polarity to delineate the effect of solvent on the optical absorption features. The perhaloporphyrins exhibit strong solvent-dependent absorption spectral features in contrast to 5,10,15,20-tetraphenylporphyrin, H2TTP. A dramatic red shift of Soret, B (>25 nm) and visible, Q (>50 nm) were observed for perhaloporphyrins in polar solvents relative to nonpolar solvents. This was ascribed to the enhanced distortion of the macrocyclic ring induced by H-bonding interaction between the porphyrin core pyrrolic N-H or pyrroline nitrogens with the solvent mols.
IT 120644-25-9, 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl- 131214-86-3, 2,3,7,8,12,13,17,18-Octabromo-5,10,15,20-tetraphenylporphyrin
RL: FRP (Properties)
(unusual solvent dependent optical absorption spectral properties of free-base perhaloporphyrins)
RN 120644-25-9 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

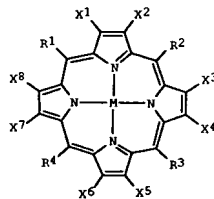


RN 131214-86-3 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



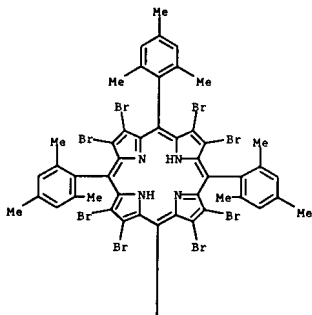
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 43 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:371490 CAPLUS
DOCUMENT NUMBER: 134:359572
TITLE: Recordable optical disk suitable for readout at 400-450 nm
INVENTOR(S): Sasa, Noboru
PATENT ASSIGNEE(S): Ricoh Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.
CODEN: JXXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:
PATENT NO. KIND DATE APPLICATION NO. DATE
JP 2001138634 A2 20010522 JP 1999-322999 19991112
PRIORITY APPL. INFO.: JP 1999-322999 19991112
OTHER SOURCE(S): MARPAT 134:359572
GI

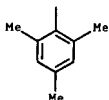


AB The invention relates to a recordable optical disk contains a novel polyolefin derivative represented by a general formula 1 (M = 2 hydrogen atoms, metal atom; X1-8 = H, F, alkyl, alkoxy; R1-4 = alicyclic substituent) in a recording layer. The recordable optical disk shows high sensitivity at a blue region.
IT 129006-48-0 139944-26-6 161405-60-3
RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)
(polyolefin derivative in recordable optical disk suitable for readout at 400-450 nm)
RN 129006-48-0 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

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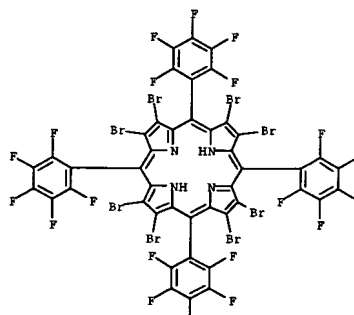


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RN 139944-26-6 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(pentafluorophenyl)-(9CI) (CA INDEX NAME)

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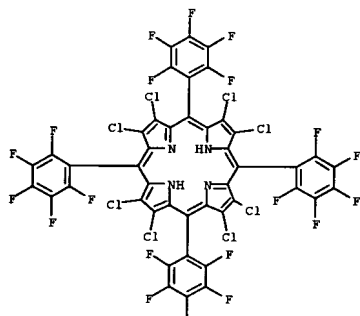


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RN 161405-60-3 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(pentafluorophenyl)-(9CI) (CA INDEX NAME)

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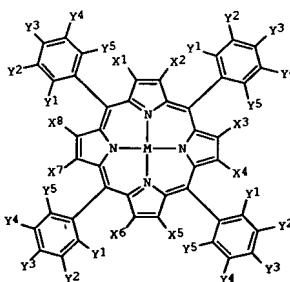


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L6 ANSWER 44 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:371489 CAPLUS
DOCUMENT NUMBER: 134:359571
TITLE: Recordable optical disk suitable for readout at 400-450 nm
INVENTOR(S): Sasa, Noboru
PATENT ASSIGNEE(S): Ricoh Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 12 pp.
CODEN: JKKXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001138633	A2	20010522	JP 1999-322756	19991112
PRIORITY APPLN. INFO.:			JP 1999-322756	19991112
OTHER SOURCE(S):			MARPAT 134:359571	

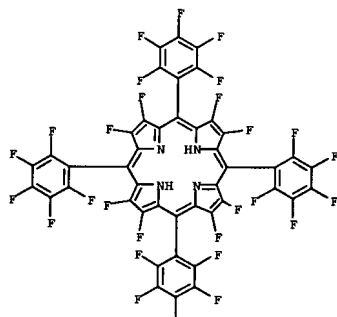


AB The invention relates to a recordable optical disk contains a novel polyolefin derivative represented by a general formula I (M = 2 hydrogen atoms, metal atoms X1-8 = H, F; Y1-5 = H, halo, nitro, cyano, OH, carbonyl, alkyl, alkoxy, aryl, amino, acyl) in a recording layer. The recordable optical disk shows high sensitivity at a blue region.

IT 121399-88-0 129006-48-0 139944-26-6
161405-60-3 166885-28-9 339274-24-7
RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)
(polyolefin derivative in recordable optical disk suitable for readout at 400-450 nm)

RN 121399-88-0 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)-(9CI) (CA INDEX NAME)

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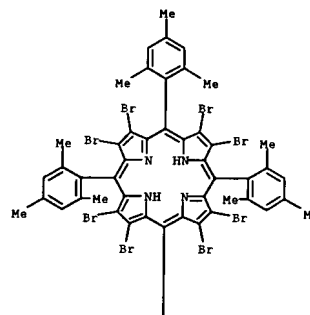


PAGE 2-A

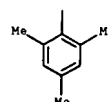


RN 129006-48-0 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

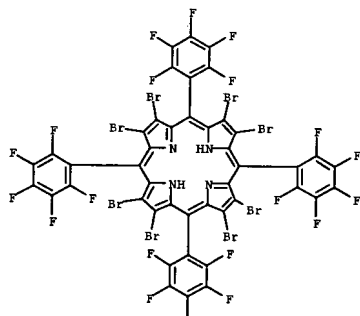


PAGE 2-A



RN 139944-26-6 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

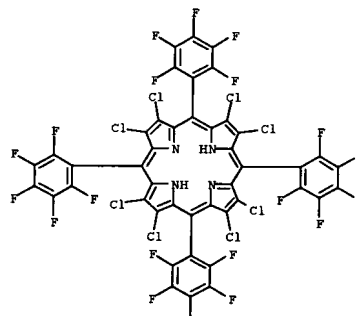


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RN 161405-60-3 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

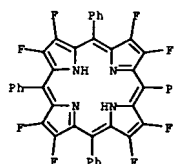
PAGE 1-A



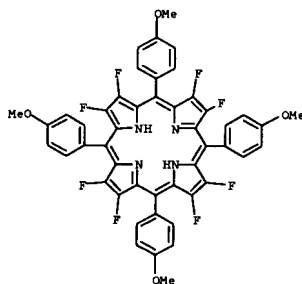
PAGE 2-A



RN 186885-28-9 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

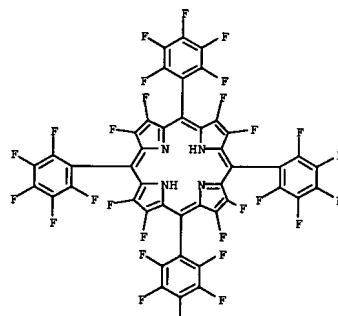


RN 339274-24-7 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



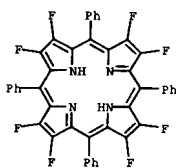
L6 ANSWER 45 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2001:294039 CAPLUS
 DOCUMENT NUMBER: 135:83504
 TITLE: Structure and Photophysics of β -Octafluoro-meso-tetraarylporphyrins
 AUTHOR(S): Smirnov, Valeriy V.; Woller, Eric K.; Tatman, Dereck; DiMauro, Stephen G.
 CORPORATE SOURCE: Department of Chemistry, University of Nebraska-Lincoln, Lincoln, NE, 68588-0304, USA
 SOURCE: Inorganic Chemistry (2001), 40(11), 2614-2619
 CODEN: INOCAJ; ISSN: 0020-1669
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The structure of THF-coordinated [2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetraphenylporphinato]zinc, Zn(F8TPP)·THF, and photophys. studies of 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetraphenylporphyrin, F8TPP, Zn(F8TPP), 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)porphyrin, F28TPP, and [2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)porphinato]zinc, Zn(F28TPP), in benzonitrile, are reported. The octafluorinated F8TPP and perfluorinated F28TPP porphyrins possess similar absorption spectra, but dissimilar x-ray crystal structures and disparate photophys. characteristics. These data cannot be easily accommodated within currently accepted theories which relate macrocycle distortion and optoelectronic properties.
 IT 121399-88-0 166885-28-9
 RL: PRP (Properties)
 (optical and photophys. properties)
 RN 121399-88-0 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

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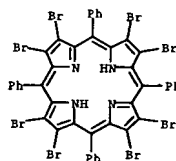
PAGE 2-A

RN 166885-28-9 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 46 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2001:85243 CAPLUS
 DOCUMENT NUMBER: 134:320094
 TITLE: Perbrominated 2-nitrotetraphenylporphyrins: electrochemical and axial ligation properties
 AUTHOR(S): Bhyrappa, Puttaiah; Purushothaman, Bhavana
 CORPORATE SOURCE: Department of Chemistry, Indian Institute of Technology-Madras, Chennai, 600 036, India
 SOURCE: Journal of the Chemical Society, Perkin Transactions 2 (2001), (2), 238-242
 CODEN: JCSPGI; ISSN: 1472-779X
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 134:320094
 AB Perbrominated 2-nitro-5,10,15,20-tetraphenylporphyrins, H2TPPBrn(NO2) (n = 6 and 7) and their metal (CuII and ZnII) complexes were synthesized and characterized. The presence of mixed electron withdrawing (bromo- and nitro-) substituents at the β -pyrrole positions induces interesting electrochem. and axial ligation properties. Perbrominated nitroporphyrins exhibit two successive one electron redox potentials with a pos. shift of >100 mV relative to their corresponding octabromotetraphenylporphyrin (MTPPBr8) complexes. Axial ligation of various nitrogenous bases to ZnTPPBrn(NO2) complexes showed facile ligand binding with >50% enhancement in the equilibrium consts., K_{eq} , relative to ZnTPPBr8. Surprisingly, MTPPBrn(NO2) complexes show similar axial ligation and electrochem. redox behavior. The anodic shift in electrochem. redox potentials and enhanced K_{eq} of MTPPBrn(NO2) complexes were attributed to the increased electron deficiency of the porphyrin π -system.
 IT 131214-86-3P
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (Preparation, electronic spectrum and electrochem. redox, and complexation with copper and zinc)
 RN 131214-86-3 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 47 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:870724 CAPLUS

DOCUMENT NUMBER: 134:222261

TITLE: Oxidation of alkanes and alkenes by iodosylbenzene and hydrogen peroxide catalyzed by halogenated manganese porphyrins in homogeneous solution and covalently bound to silica

AUTHOR(S): Doro, F. G.; Smith, J. R. L.; Ferreira, A. G.; Assis, M. D.

CORPORATE SOURCE: Departamento de Quimica, Universidade de Sao Paulo, Faculdade de Filosofia Ciencias e Letras de Ribeirao Preto, Ribeirao Preto, Sao Paulo, 14040-901, Brazil

SOURCE: Journal of Molecular Catalysis A: Chemical (2000), 164(1-2), 97-108

CODEN: JMCCF2; ISSN: 1381-1169

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:222261

AB Manganese(III) 5-(pentafluorophenyl)-10,15,20-tri(2,6-dichlorophenyl)porphyrin, Mn(PFTDCPP), and manganese(III) 2,3,7,8,12,13,17,18-octachloro-5-(pentafluorophenyl)-10,15,20-tri(2,6-dichlorophenyl)porphyrin, Mn(PFTDCC18PP), have been synthesized and used as catalysts in hydrocarbon oxidations by iodosylbenzene and hydrogen peroxide both in solution and covalently bound to aminopropylated silica. The former shows higher efficiency in the epoxidation of alkenes by iodosylbenzene, whereas the perchlorinated manganese porphyrin is more efficient in the hydroxylation of alkanes by this oxidant. The supported manganese(III) porphyrin show the same activity as its homogeneous analog. With hydrogen peroxide as oxygen donor, Mn(PFTDCPP) is a stable and effective catalyst in the presence of imidazole. The perchlorinated analog is a poor catalyst with this oxidant. The eight additional chlorine atoms on the porphyrin ring stabilize Mn(II) and unfavour the formation of the active species, MnV=O.

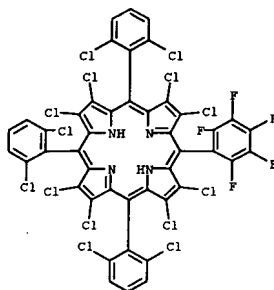
IT 328897-67-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(oxidation of alkanes and alkenes by iodosylbenzene and hydrogen peroxide catalyzed by halogenated manganese porphyrins in homogeneous solution and covalently bound to silica)

RN 328897-67-2 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15-tris(2,6-dichlorophenyl)-20-(pentafluorophenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 47 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



REFERENCE COUNT: 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 48 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:802778 CAPLUS

DOCUMENT NUMBER: 134:100852

TITLE: Direct Synthesis of Expanded Fluorinated Calix[n]pyrroles: Decafluorocalix[5]pyrrole and Hexadecafluorocalix[8]pyrrole

AUTHOR(S): Sessler, Jonathan L.; Anzenbacher, Pavel, Jr.; Shriver, James A.; Jursikova, Karolina; Lynch, Vincent M.; Marquez, Manuel

CORPORATE SOURCE: Department of Chemistry and Biochemistry and Institute for Cellular and Molecular Biology, University of Texas at Austin, Austin, TX, 78712-1167, USA

SOURCE: Journal of the American Chemical Society (2000), 122(48), 12061-12062

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:100852

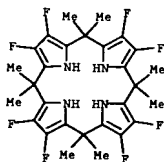
AB Methanesulfonic acid-catalyzed condensation of 3,4-difluoropyrrole and acetone gives, in addition to octafluorocalix[4]pyrrole, the dominant reaction product, appreciable quantities of both the corresponding calix[5] and calix[8] products.

IT 311804-81-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of fluorinated calix[n]pyrroles)

RN 311804-81-6 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 49 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:735661 CAPLUS

DOCUMENT NUMBER: 134:91666

TITLE: Metalloporphyrin catalytic oxidations of hydrocarbons by H2O2

AUTHOR(S): Rocha Gonsalves, Antonio M. d'A.; Serra, Armenio C.

CORPORATE SOURCE: Departamento de Quimica, Universidade de Coimbra, Coimbra, P-3049, Port.

SOURCE: Journal of Porphyrins and Phthalocyanines (2000), 4(6), 598-603

CODEN: JPPHFZ; ISSN: 1088-4246

PUBLISHER: John Wiley & Sons Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The metalloporphyrin catalytic oxidation of hydrocarbons using dilute

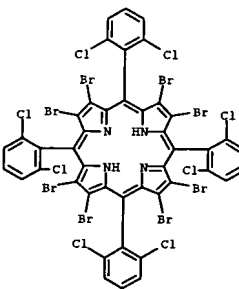
hydrogen peroxide as oxygen donor with a two-phase system in the presence of an excess of benzoic acid is studied. Porphyrins derived from meso-tetrakis(2,6-dichlorophenyl)porphyrin and bearing sulfonamide substituents at β or meso positions and halogens at β positions were used. The system allowed for very efficient catalytic epoxidations and hydroxylations of hydrocarbons. It is proved that the excess of benzoic acid is critical to the catalyst efficiency and stability. The role of the lipophilic acid in this system is discussed.

IT 107035-95-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(metalloporphyrin catalytic oxidations of hydrocarbons by H2O2)

RN 107035-95-0 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,6-dichlorophenyl)- (9CI) (CA INDEX NAME)

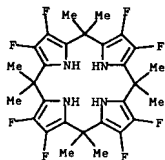


REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 50 OF 148 CAPLUS COPYRIGHT 2005 ACS ON STN
 ACCESSION NUMBER: 2000:707590 CAPLUS
 DOCUMENT NUMBER: 134:29395
 TITLE: Fluorinated Calix[4]pyrrole and Dipyrrolylquinoxaline:
 Neutral Anion Receptors with Augmented Affinities and
 Enhanced Selectivities
 AUTHOR(S): Anzenbacher, Pavel, Jr.; Try, Andrew C.; Miyaji,
 Hidekazu; Jursikova, Karolina; Lynch, Vincent M.;
 Marquez, Manuel; Sessler, Jonathan L.
 CORPORATE SOURCE: Department of Chemistry and Biochemistry and Institute
 for Cellular and Molecular Biology, University of
 Texas at Austin, Austin, TX, 78712-1167, USA
 SOURCE: Journal of the American Chemical Society (2000),
 122(42), 10268-10272
 CODEN: JACSAT; ISSN: 0002-7863
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

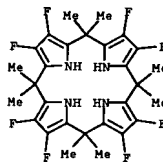
AB Octamethyloctafluorocalix[4]pyrrole and 2,3-di(3,4-difluoropyrrol-2-yl)quinoxaline were prepared from 3,4-difluoro-1H-pyrrole. These latter two entities act as neutral anion receptors and bind anions such as fluoride, chloride, or dihydrogen phosphate with an enhanced affinity compared to their non-fluorinated congeners as judged from ¹H NMR, ¹⁹F NMR, and fluorescence emission spectroscopic analyses. The increase in affinity was especially high in case of chloride and dihydrogen phosphate anion, with the 2,3-di(3,4-difluoropyrrol-2-yl)quinoxaline system, in particular, displaying an affinity for H₂PO₄⁻ that was improved by 3 orders of magnitude as compared to its non-fluorinated congener. This improvement in the affinity for the dihydrogen phosphate is accompanied by change of color from pale yellow to orange, thus allowing the use of such compds. as naked-eye sensors for phosphate anion. In the case of the octafluorocalix[4]pyrrole system X-ray diffraction analyses revealed the presence of four different macrocyclic conformations in the solid state, as well as close intermol. contacts mediated by apparent CF...HN hydrogen bonds.

IT 311804-81-6P
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (Preparation and anion binding by octafluorooctamethylcalixpyrrole and bis(difluoropyrrolyl)quinoxaline)
 RN 311804-81-6 CAPLUS
 CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)

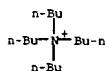


IT 311804-87-2P 311804-88-3P 311804-89-4P
 311804-94-1P

L6 ANSWER 50 OF 148 CAPLUS COPYRIGHT 2005 ACS ON STN (Continued)
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and anion binding by octafluorooctamethylcalixpyrrole and bis(difluoropyrrolyl)quinoxaline)
 RN 311804-87-2 CAPLUS
 CN 1-Butanammonium, N,N,N-tributyl-, fluoride, compd. with
 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)
 CM 1
 CRN 311804-81-6
 CMF C28 H28 F8 N4



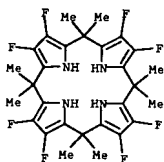
CM 2
 CRN 429-41-4
 CMF C16 H36 N . F



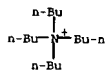
● F⁻

RN 311804-88-3 CAPLUS
 CN 1-Butanammonium, N,N,N-tributyl-, chloride, compd. with
 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)
 CM 1
 CRN 311804-81-6
 CMF C28 H28 F8 N4

L6 ANSWER 50 OF 148 CAPLUS COPYRIGHT 2005 ACS ON STN (Continued)

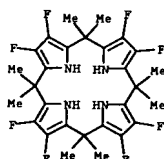


CM 2
 CRN 1112-67-0
 CMF C16 H36 N . Cl



● Cl⁻

RN 311804-89-4 CAPLUS
 CN 1-Butanammonium, N,N,N-tributyl-, phosphate, compd. with
 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl-21H,23H-porphine (1:1) (9CI) (CA INDEX NAME)
 CM 1
 CRN 311804-81-6
 CMF C28 H28 F8 N4



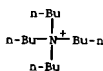
CM 2

L6 ANSWER 50 OF 148 CAPLUS COPYRIGHT 2005 ACS ON STN (Continued)
 CRN 5574-97-0
 CMF C16 H36 N . H2 O4 P

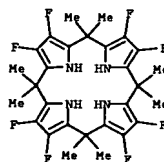
CM 3
 CRN 14066-20-7
 CMF H2 O4 P



CM 4
 CRN 10549-76-5
 CMF C16 H36 N



RN 311804-94-1 CAPLUS
 CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl-, compd. with
 sulfanylbis(methane) (1:1) (9CI) (CA INDEX NAME)
 CM 1
 CRN 311804-81-6
 CMF C28 H28 F8 N4



CM 2
 CRN 67-68-5
 CMF C2 H6 O S



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

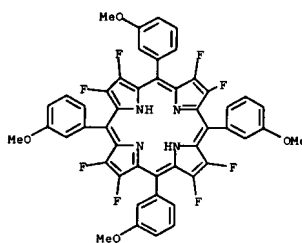
L6 ANSWER 51 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2000:680398 CAPLUS
 DOCUMENT NUMBER: 133:252219
 TITLE: synthesis of octafluoro-meso-tetraarylporphyrins and their metal complexes for use as catalysts
 INVENTOR(S): Dimagno, Stephen G.
 PATENT ASSIGNEE(S): University of Nebraska-Lincoln, USA
 SOURCE: U.S., 10 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6124452	A	20000926	US 1997-994891	19971219
PRIORITY APPL. INFO.:			US 1997-994891	19971219
OTHER SOURCE(S):			CASREACT 133:252219; MARPAT 133:252219	

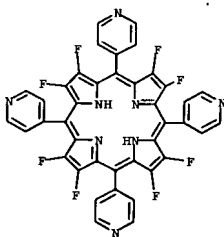
AB The title compds. are synthesized by reacting 3,4-difluoropyrrole with an aromatic aldehyde in the presence of boron trifluoride etherate, followed by oxidation. The difluoropyrrole used in this reaction is produced by reacting 3,3,4,4-tetrafluoropyrrolidine or its corresponding salt, with a base such as potassium tert-butoxide. The metalloporphyrins of the present invention are synthesized by deprotonating β -octafluoro-meso-tetraarylporphyrin ligands and treating said ligands with metal ions.

IT 186885-29-OP 295778-60-SP
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
 (synthesis of octafluoro-meso-tetraarylporphyrins and their metal complexes for use as catalysts)

RN 186885-29-0 CAPLUS
 CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(3-methoxyphenyl)- (9CI) (CA INDEX NAME)



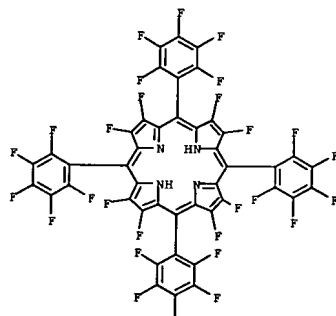
RN 295778-60-8 CAPLUS
 CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetra-4-pyridinyl- (9CI) (CA INDEX NAME)



IT 121399-88-OP 186885-28-SP
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (synthesis of octafluoro-meso-tetraarylporphyrins and their metal complexes for use as catalysts)

RN 121399-88-0 CAPLUS
 CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

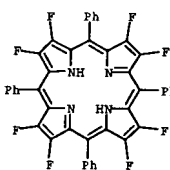
PAGE 1-A



PAGE 2-A

F

RN 186885-28-9 CAPLUS
 CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

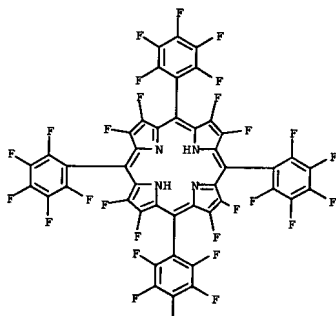
L6 ANSWER 52 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2000:570824 CAPLUS
 DOCUMENT NUMBER: 133:296117
 TITLE: Umpolung of a Metal-Carbon Bond: A Potential Route to Porphyrin-Based Methane Functionalization Catalysts
 AUTHOR(S): Nelson, Andrew P.; DiMaggio, Stephen G.
 CORPORATE SOURCE: Department of Chemistry, University of Nebraska-Lincoln, Lincoln, NE, 68588-0304, USA
 SOURCE: Journal of the American Chemical Society (2000), 122(35), 8569-8570
 CODEN: JACSAT; ISSN: 0002-7863
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB A modified Rh porphyrin complex performs each of the reactions in a formal catalytic cycle involved in converting methane, triphenylphosphine, and strong acid to a methylphosphonium salt and dihydrogen. The key design principle, that ligand modification can so increase metal nucleofugacity that nucleophilic substitution can be activated without compromising alkane and H activation, is drawn directly from fundamental concepts of chemical bonding. Developing an efficient catalytic system from these or similar components requires dramatically accelerated rates of the methane activation and nucleophilic functionalization.

IT 121399-88-0
 RL: CAT (Catalyst use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
 (ligands: umpolung of metal-carbon bond and route to porphyrin-based methane functionalization catalysts)

RN 121399-88-0 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

PAGE 1-A



L6 ANSWER 52 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 2-A

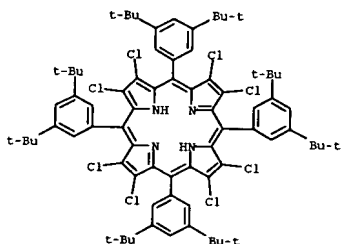
REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 53 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2000:472188 CAPLUS
 DOCUMENT NUMBER: 133:202236
 TITLE: Halogenation of metalloporphyrins
 AUTHOR(S): Rumsantseva, V. D.; Aksenova, E. A.; Ponamareva, O. N.; Mironov, A. F.
 CORPORATE SOURCE: Lomonosov State Academy of Fine Chemical Technology, Moscow, 117571, Russia
 SOURCE: Russian Journal of Bioorganic Chemistry (Translation of Bioorganicheskaya Khimiya) (2000), 26(6), 423-428
 CODEN: RJBCET; ISSN: 1068-1620
 PUBLISHER: MAIK Nauka/Interperiodica
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Thionyl chloride can chlorinate porphyrin complexes with transient metals (Pd, Ni, or Cu) at the free β and meso-positions of the porphyrin macrocycle. A more prolonged or rigorous treatment also causes the chlorination of side alkyl substituents, mainly, Me groups.

IT 288843-06-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation from chlorination of metalloporphyrins)

RN 288843-06-1 CAPLUS
 CN 21H,23H-Porphine, 5,10,15,20-tetrakis[3,5-bis(1,1-dimethylethyl)phenyl]-2,3,7,8,12,13,17,18-octachloro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

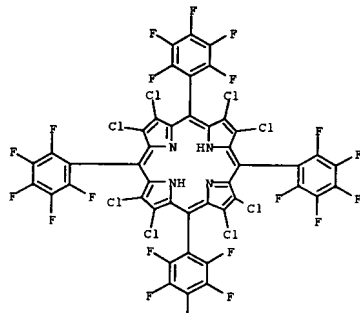
L6 ANSWER 54 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2000:426679 CAPLUS
 DOCUMENT NUMBER: 133:266543
 TITLE: The oxidation of ethylbenzene and other alkylaromatics by dioxigen catalyzed by iron(III) tetrakis(pentafluorophenyl)porphyrin and related iron porphyrins
 AUTHOR(S): Evans, Steven; Lindsay Smith, John R.
 CORPORATE SOURCE: Department of Chemistry, University of York, York, YO10 5DD, UK
 SOURCE: Perkin 2 (2000), (7), 1541-1552
 CODEN: PRKTF0
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 133:266543
 AB The oxidation of ethylbenzene with dioxigen catalyzed by iron(III) porphyrins

in a solvent free system was studied over the temperature range 30-110 °C. The time dependence of the formation of the three main products, 1-phenylethanol, acetophenone and 1-phenylethyl hydroperoxide, and the fate of the iron porphyrin are interpreted in terms of a free radical autoxidn. mechanism. The yields of the oxidation products are determined by the rate of reaction and by the lifetime of the catalyst. Catalyst degradation is shown to involve reaction of the porphyrin ligand with 1-phenylethoxyl and 1-phenylethylperoxyl radicals. The disadvantages of increased induction periods and longer reaction times of the oxidns. observed

at lower reaction temps. are counter balanced by increased catalyst turnovers. Less extensive studies on the oxidns. of toluene, cumene, (2-methylpropyl)benzene and tert-butylbenzene support the overall mechanism proposed for ethylbenzene. A comparative study using the catalysts iron(III) 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(2,6-dichlorophenyl)porphyrin and iron(III) tetrakis(pentafluorophenyl)porphyrin and five of its derivate. reveals that halogenation of the β -pyrrole positions markedly increases the activity of the catalysts but not the stability of the porphyrin towards degradation. The highest yields were obtained with the μ -oxo dimer of iron(III) tetrakis(pentafluorophenyl)porphyrin and iron(III) tetrakis(4-dimethylamino-2,3,5,6-tetrafluorophenyl)porphyrin.

IT 161405-60-3P, 2,3,7,8,12,13,17,18-Octachloro-5,10,15,20-tetrakis(pentafluorophenyl)-21H,23H-Porphine
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (oxidation of (alkyl)benzenes by dioxigen catalyzed by iron porphyrins)
 RN 161405-60-3 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

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REFERENCE COUNT: 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2000:417208 CAPLUS
DOCUMENT NUMBER: 133:213839
TITLE: Mechanistic Studies of (Porphinato)Iron-Catalyzed Isobutane Oxidation. Comparative Studies of Three Classes of Electron-Deficient Porphyrin Catalysts
AUTHOR(S): Moore, Kevin T.; Horvath, Istvan T.; Therien, Michael J.
CORPORATE SOURCE: Department of Chemistry, University of Pennsylvania, Philadelphia, PA, 19104-6323, USA
SOURCE: Inorganic Chemistry (2000), 39(15), 3125-3139
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

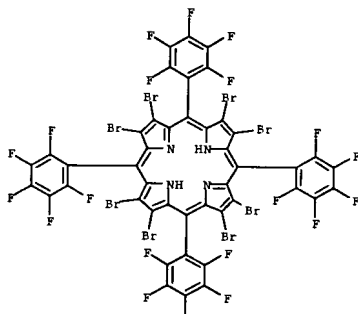
AB We report herein a comprehensive study of (porphinato)iron (PFe)-catalyzed isobutane oxidation in which mol. oxygen is utilized as the sole oxidant; these catalytic reactions were carried out and monitored in both autoclave reactors and sapphire NMR tubes. In situ ¹⁹F and ¹³C NMR expts., coupled with GC analyses and optical spectra obtained from the autoclave reactions have enabled the identification of the predominant porphyrinic species present during PFe-catalyzed oxidation of isobutane. Electron-deficient PFe catalysts based on 5,10,15,20-tetrakis(pentafluorophenyl)porphyrin [(C6F₅)₄PH₂], 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(pentafluorophenyl)porphyrin (Br₈(C6F₅)₄PH₂), and 5,10,15,20-tetrakis(heptafluoropropyl)porphyrin [(C3F₇)₄PH₂] macrocycles were examined. The nature and distribution of hydrocarbon oxidation products show that an autoxidn. reaction pathway dominates the reaction kinetics, consistent with a radical chain process. For each catalytic system examined, PFeII species were shown not to be stable under moderate O₂ pressure at 80 °C; in every case, the PFeII catalyst precursor was converted quant. to high-spin PFeIII complexes prior to the observation of any hydrocarbon oxidation products. Once catalytic isobutane oxidation is initiated, all reactions are marked by concomitant decomposition of the porphyrin-based catalyst. In situ ¹⁷O NMR spectroscopic studies confirm the incorporation of ¹⁷O from labeled water into the oxidation products, implicating the involvement of PFe-OH in the catalytic cycle. Importantly, Br₈(C6F₅)₄PFe-based catalysts, which lack macrocycle C-H bonds, do not exhibit augmented stability with respect to analogous catalysts based on (C6F₅)₄PFe and (C3F₇)₄PFe species. The data presented are consistent with a hydrocarbon oxidation process in which PFe complexes play dual roles of a radical chain initiator, and the species responsible for the catalytic decomposition of organic peroxides. This modified Haber-Weiss reaction scheme provides for the decomposition of tert-Bu hydroperoxide intermediates via reaction with PFe-OH complexes; the PFeIII species responsible for hydroperoxide decomposition are regenerated by reaction of PFeII with dioxygen under these exptl. conditions.

IT 139944-26-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(studies of (porphinato)iron-catalyzed isobutane oxidation)

RN 139944-26-6 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

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REFERENCE COUNT: 94 THERE ARE 94 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

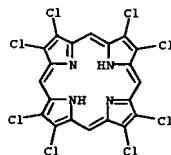
ACCESSION NUMBER: 2000:282110 CAPLUS
DOCUMENT NUMBER: 133:43367
TITLE: Triplet Excited States of Free-Base Porphin and Its β -Octahalogenated Derivatives
AUTHOR(S): Nguyen, Kiet A.; Day, Paul N.; Pachter, Ruth
CORPORATE SOURCE: Air Force Research Laboratory, Materials and Manufacturing Directorate AFRL/MLPJ, Wright-Patterson Air Force Base, OH, 45433-7702, USA
SOURCE: Journal of Physical Chemistry A (2000), 104(20), 4748-4754
CODEN: JPCAPH; ISSN: 1089-5639
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB D. functional theory (DFT) electronic structure calcns. were carried out to predict the structures, energetics, and triplet-triplet (T-T) spectra for the low-lying triplet states of free-base porphin (PH₂) and its β -octahalogenated derivs. (β -PH₂X₈; X = F, Cl, Br). The lowest triplet excited state of PH₂ and β -PH₂X₈ was found to retain D_{2h} symmetry with stretched C β -C β and C β -C α bond distances. For free-base porphin, the singlet-triplet (S₀-T₁) gap obtained with the B3LYP functional was in excellent agreement with the exptl. phosphorescence value. Excitation energies computed by time-dependent DFT also provided a fine account of the observed T-T spectrum. β -Halogenation had little effect on the singlet-triplet gaps of porphins. The S₀-T₁ and S₀-T₂ splittings for β -PH₂X₈ were within 0.1 eV of the corresponding splittings in the unsubstituted porphin. All bands in the T-T spectra of β -PH₂X₈ were predicted to be significantly (up to 0.65 eV) red-shifted in comparison to corresponding bands of the unsubstituted porphin.

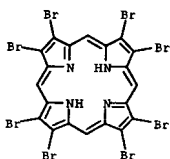
IT 144811-81-4, Octachloroporphine 144811-83-6, Octabromoporphine 144811-86-9, Octafluoroporphine
RL: FRP (Properties)
(triplet excited states of free-base porphine and its β -octahalogenated derivs.)

RN 144811-81-4 CAPLUS

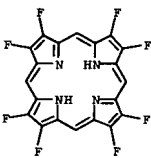
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro- (9CI) (CA INDEX NAME)



RN 144811-83-6 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo- (9CI) (CA INDEX NAME)



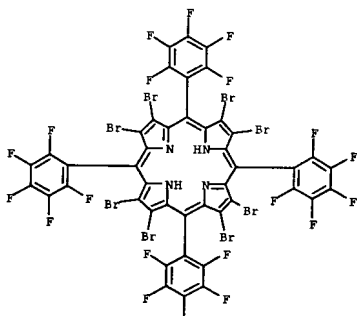
RN 144811-86-9 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 57 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:770768 CAPLUS
DOCUMENT NUMBER: 132:129866
TITLE: Photocatalytic activation of oxygen by iron(III) porphyrins
AUTHOR(S): Hennig, Horst; Lippa, Doritt
CORPORATE SOURCE: Institut für Anorganische Chemie, Universität Leipzig, Leipzig, D-04103, Germany
SOURCE: Journal fuer Praktische Chemie (Weinheim, Germany) (1999), 341(8), 757-767
CODEN: JPCHP4; ISSN: 1436-9966
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: German
AB Photochem. charge transfer excitation of tetraphenyl(porphyrinato)iron(III) complexes yields tetraphenyl(porphyrinato)iron(II) which is able to coordinate O₂ under formation of oxo-[tetraphenyl(porphyrinato)iron(IV)]. Based on this photochem. reaction pathway photocatalytic oxygenation of α-pinene and other alkenes can be initiated. Fe(III) complexes of tetramesitylporphyrin, tetrakis(pentafluorophenyl)porphyrin, octa-β-bromo-tetrakis(pentafluorophenyl)porphyrin, and octa-β-chloro-tetrakis(pentafluorophenyl)porphyrin were investigated photochem. with the aim to improve the low photochem. efficiency of tetraphenyl(porphyrinato)iron(III). The influence of substituents on the porphyrin ligand on the photochem. behavior of the corresponding Fe(III) complexes is measured mainly by temperature dependent UV/Vis spectroscopy. Both, the yield of oxygenation products formed photocatalytically with α-pinene and the product distribution (allylic alcs. vs. epoxide) depend on the design of the porphyrin ligands coordinated with Fe(III).
IT 139944-26-6 161405-60-3
RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of Fe(III) porphyrin complexes)
RN 139944-26-6 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

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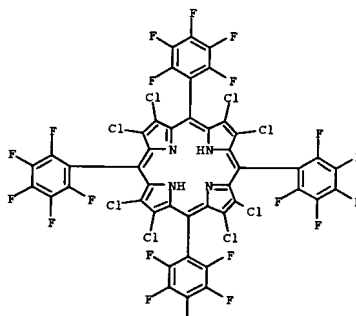


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RN 161405-60-3 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

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REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

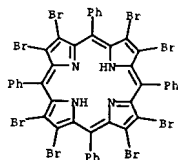
L6 ANSWER 58 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:770348 CAPLUS
DOCUMENT NUMBER: 132:92953
TITLE: Electronic effects on the stereoselectivity of epoxidation reactions catalyzed by manganese porphyrins
AUTHOR(S): Baciocchi, Enrico; Boschi, Tristano; Cassioli, Luigi; Galli, Carlo; Jaquinod, Laurent; Lapi, Andrea; Paolesse, Roberto; Smith, Kevin M.; Tagliatesta, Pietro
CORPORATE SOURCE: Dipartimento Chimica, Univ. La Sapienza, Rome, I-00185, Italy
SOURCE: European Journal of Organic Chemistry (1999), (12), 3281-3286
CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A series of Mn(III) porphyrins progressively halogenated in the β -pyrrolic positions was employed to catalyze the epoxidn. of cis-stilbene by iodosylbenzene, and to study the role of the electronic effects on the stereoselectivity of this process. A gradual improvement in the stereoselectivity on increasing the number of β -halogen atoms was observed. The role of steric effects upon the epoxidn. was also investigated by placing ortho-substituents in the meso-Ph rings, and it was found that steric effects are more important than electronic effects toward the stereoselectivity of this process. These results can be rationalized by proposing a competition between a non-stereoselective electrophilic pathway of addition and a stereospecific pathway of O insertion, the former being disfavored by electron-withdrawing substituents. Alternatively, the formation of an open intermediate between the Mn(V) oxene and the substrate could be suggested, where the stereoselectivity ought to be determined by the competition between closure of the epoxide ring and rotation around the C-C bond. In this case, the enhanced stereoselectivity given by our polyhalogenated porphyrins might be attributed to an acceleration of the epoxide ring closure caused by the electron-withdrawing effect of the halogen substituents.

IT 131214-86-3
RL: RCT (Reactant); RACT (Reactant or reagent) (coordination; steric and electronic substituent effects of porphyrin ligands on Mn porphyrin-catalyzed stereoselective epoxidn. of cis-stilbene)

RN 131214-86-3 CAPLUS
CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

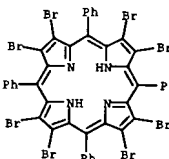


L6 ANSWER 58 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 59 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

Cl
Cl-CH-Cl
CH 2
CRN 161614-77-3
CMF C44 H22 Br8 N4 . 2 C2 H F3 O2
CH 3
CRN 131214-86-3
CMF C44 H22 Br8 N4



CH 4
CRN 76-05-1
CMF C2 H F3 O2



IT 161614-77-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (crystal structure and conformation of porphyrin dications)
RN 161614-77-3 CAPLUS
CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,13,20-tetraphenyl-, bis(trifluoroacetate), compd. with trichloromethane (2:1) (9CI) (CA INDEX NAME)

CH 1
CRN 131214-86-3
CMF C44 H22 Br8 N4

L6 ANSWER 59 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN

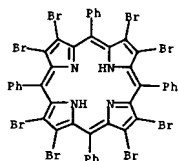
ACCESSION NUMBER: 1999:529518 CAPLUS
DOCUMENT NUMBER: 131:351141
TITLE: Structure and conformation of tetra-meso-, octa- β -, and dodeca-substituted 22,24-dihydroporphyrins (porphyrin dications)
AUTHOR(S): Senge, Mathias O.; Kalisch, Werner W.
CORPORATE SOURCE: Institut Chemie, Organische Chemie, Freie Univ. Berlin, Berlin, D-14195, Germany
SOURCE: Zeitschrift fuer Naturforschung, B: Chemical Sciences (1999), 54(7), 943-959
CODEN: ZNBSEN; ISSN: 0932-0776
PUBLISHER: Verlag der Zeitschrift fuer Naturforschung
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A comparative crystallog. anal. of the conformation of porphyrin diacids with various substituent types reveals considerable differences in the degree of nonplanarity and distortion modes. Diacids of 5,10,15,20-tetraarylporphyrins generally exhibit typical saddle-distorted macrocycles with displacements of the C β positions in the range of 0.7-1.0 Å. Adding peripheral substituents, i.e., using dodeca-substituted porphyrins for the diacid formation yields similar distortion types albeit with larger out-of-plane displacements. As a result of the combined effect of both peripheral (interaction between the C β and C α substituents) and core (interaction between the 4 inner H atoms) steric strain the maximum C β displacements reach 1.3-1.5 Å. Quite a different situation is observed for the diacids of 2,3,7,8,12,13,17,18-octaalkylporphyrins. Here, macrocycles with pair-wise displacement of neighboring pyrrole rings and significant NH pyramidalization and those with classic saddle distortion are found. Generally, octa- β -substituted porphyrin diacids show smaller degrees of nonplanarity; C β displacements ranged from 0.6 to 0.72 Å. On the basis of the overall degree of conformational distortion ($\Delta 24$ = average deviation of the 24 macrocycles atoms from the mean plane), the 3 different types of porphyrin macrocycles studied differ considerably in their degree of conformational flexibility. For several porphyrin crystal structures with different counterions and/or solvate molcs. were obtained. Taking into account results from the literature, 2,3,7,8,12,13,17,18-octaethyl-22,24-dihydro-5,10,15,20-tetraphenylporphyrin shows the smallest degree of flexibility ($\Delta 24$ = 0.61-0.63 Å; 4 different x-ray structures), while 22,24-dihydro-5,10,15,20-tetraphenylporphyrin is more flexible ($\Delta 24$ = 0.42-0.52 Å; 4 structures). The largest flexibility is observed for 2,3,7,8,12,13,17,18-octaethyl-22,24-dihydroporphyrin ($\Delta 24$ = 0.02-0.33 Å; 4 structures).

IT 161614-78-4
RL: PRP (Properties) (crystal structure)

RN 161614-78-4 CAPLUS
CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,13,20-tetraphenyl-, bis(trifluoroacetate), compd. with trichloromethane (2:1) (9CI) (CA INDEX NAME)

CH 1
CRN 67-66-3
CMF C H Cl3



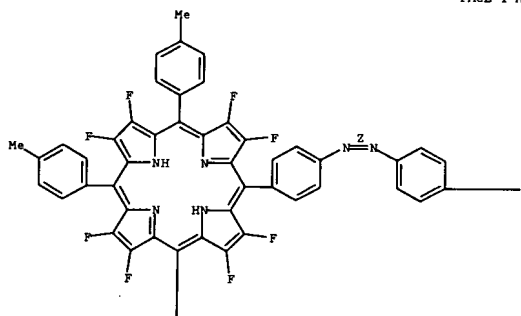
CH 2
CRN 76-05-1
CHF C2 H F3 O2



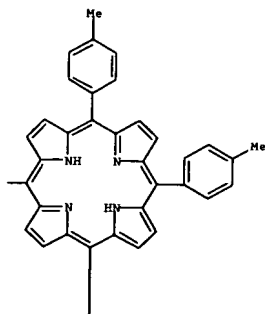
REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 60 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:525327 CAPLUS
DOCUMENT NUMBER: 131:329692
TITLE: Intramolecular Electron Transfer of Diporphyrins Comprised of Electron-Deficient Porphyrin and Electron-Rich Porphyrin with Photocontrolled Isomerization. (Erratum to document cited in CA130:160405)
AUTHOR(S): Tsuchiya, Shinji
CORPORATE SOURCE: Institute Industrial Science, Univ. Tokyo, Tokyo, 106, Japan
SOURCE: Journal of the American Chemical Society (1999), 121(35), 8132
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The first two sentences in Reference 41 on page 6521 should be the following:
"(41) the syntheses of β -octafluorinated porphyrins using 3,4-difluoropyrrole as a precursor have been reported by DiMaggio and Leroy. The compds. obtained from the 3,4-difluoropyrrole route have different phys. properties than those reported in reference 7 of J. Am. Chemical Society 1999, 121, 48-53."
IT 220213-35-4
RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); FORM (Formation, nonpreparative); PROC (Process)
(fluorescence and photoisomerization and photoinduced intramol. electron-transfer of azobenzene-linked diporphyrin Zn complexes and free base analogs (Erratum) (Erratum))
RN 220213-35-4 CAPLUS
CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15-tris(4-methylphenyl)-20-[4-[(1Z)-[4-{10,15,20-tris(4-methylphenyl)-21H, 23H-porphin-5-yl]phenyl]azo]phenyl]- (9CI) (CA INDEX NAME)
Double bond geometry as shown.

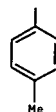
PAGE 1-A



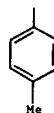
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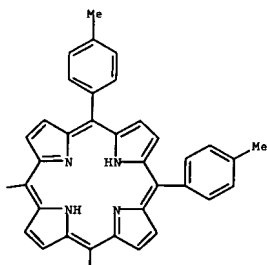


IT 220213-34-3P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(fluorescence and photoisomerization and photoinduced intramol. electron-transfer of azobenzene-linked diporphyrin Zn complexes and free base analogs (Erratum) (Erratum))
RN 220213-34-3 CAPLUS
CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15-tris(4-methylphenyl)-20-[4-[(1E)-[4-{10,15,20-tris(4-methylphenyl)-21H, 23H-porphin-5-yl]phenyl]azo]phenyl]- (9CI) (CA INDEX NAME)
Double bond geometry as shown.

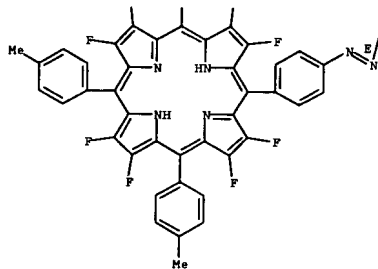
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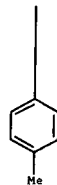
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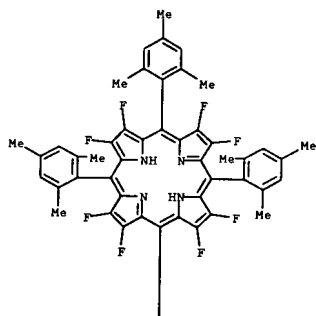


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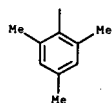


IT 220213-36-5
 RL: PRP (Properties)
 (fluorescence quenching by electron transfer from electron-rich to
 electron-deficient porphyrin in relation to photophysics of
 azobenzene-linked diporphyrins (Erratum) (Erratum))
 RN 220213-36-5 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(2,4,6-
 trimethylphenyl)- (9CI) (CA INDEX NAME)

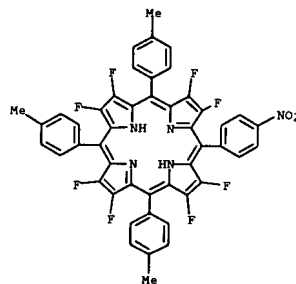
PAGE 1-A



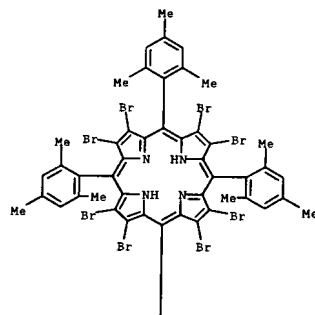
PAGE 2-A



IT 220213-37-6
 RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
 (in synthesis of azobenzene-linked diporphyrin Zn complexes (Erratum)
 (Erratum))
 RN 220213-37-6 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15-tris(4-
 methylphenyl)-20-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



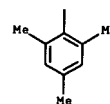
L6 ANSWER 61 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1999:523271 CAPLUS
 DOCUMENT NUMBER: 131:299306
 TITLE: Novel dodecaarylporphyrins: synthesis and dynamic properties
 AUTHOR(S): Muzzi, Cinzia M.; Medforth, Craig J.; Voss, Lisa; Cancilla, Mark; Lebrilla, Carlito; Ma, Jian-Guo; Shelmutt, John A.; Smith, Kevin M.
 CORPORATE SOURCE: Department of Chemistry, University of California, Davis, CA, 95616, USA
 SOURCE: Tetrahedron Letters (1999), 40(34), 6159-6162
 CODEN: TELEAY; ISSN: 0040-4039
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 131:299306
 AB An investigation of the synthesis of dodecaarylporphyrins using the Suzuki coupling reaction of arylboronic acids with octabromotetraarylporphyrins is reported. Variable temperature ¹H NMR studies of these new porphyrins reveal several dynamic processes including the 1st examples of β-aryl rotation.
 IT 129006-48-0 131214-86-3 139944-26-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reactant for preparation of dodecaarylporphyrins)
 RN 129006-48-0 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)



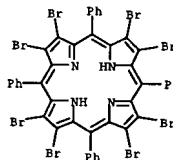
PAGE 1-A

L6 ANSWER 61 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 2-A

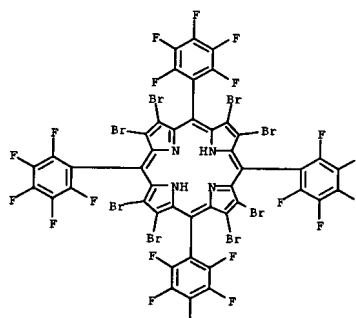


RN 131214-86-3 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



RN 139944-26-6 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

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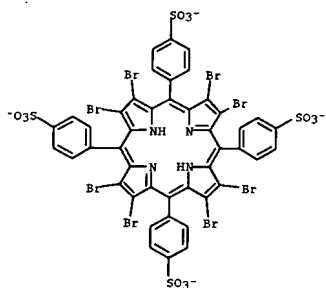


L6 ANSWER 61 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

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REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

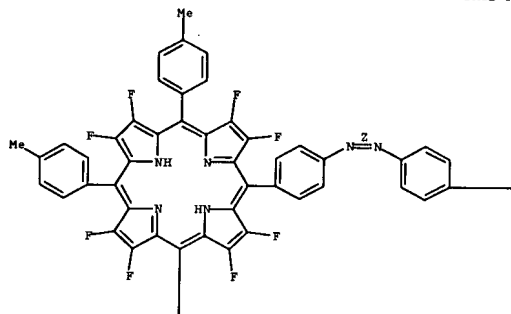
L6 ANSWER 62 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1999:416534 CAPLUS
 DOCUMENT NUMBER: 131:96507
 TITLE: Separation and transport of lithium of 10-5 M in the presence of sodium chloride higher than 0.1 M by 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(4-sulfonatophenyl)porphyrin
 AUTHOR(S): Sun, Haiping; Tabata, Masaaki
 CORPORATE SOURCE: Department of Chemistry, Faculty of Science and Engineering, Saga University, Saga, 840-8502, Japan
 SOURCE: Talanta (1999), 49(3), 603-610
 CODEN: TALNTA; ISSN: 0039-9140
 PUBLISHER: Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A water-soluble porphyrin (2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(4-sulfonatophenyl)porphyrin (H2(obtpps)4-, H2P4-)) synthesized in the laboratory was applied to a solvent extraction method and a liquid membrane transport of lithium ≥10-5 M (M = mol dm-3) in the presence of sodium chloride >0.1 M. The lithium porphyrin with five neg. charges was extracted successfully into chloroform with tetrabutylammonium ion ((Me3C)4N+) at pH 12.7. The extraction constant for the reaction of [LiP5-]a + 5[(Me3C)4N]o+ ·d.b.h.w. [((Me3C)4N)5LiP]o is (1.9 ± 0.3) + 1018 M-5, where the subscripts a and o denote chemical species in aqueous and organic phases, resp. Lithium was transported to an aqueous phase at pH 7 through a chloroform liquid membrane containing [((Me3C)4N)5HP]. The extraction and transport mechanism was discussed from extraction const., chemical species and transportation rate. Lithium in sea water or serum sample was separated and its concentration was determined spectrophotometrically by the present method without any interference from sodium chloride. The interference from transition and heavy metal ions was masked by Mg-EDTA. A calibration curve was linear at 2 + 10-6-2 + 10-5 M at a precision of 1.51% (relative standard deviation).
 IT 176173-80-1, 2,3,7,8,12,13,17,18-Octabromo-5,10,15,20-tetrakis(4-sulfonatophenyl)porphyrin
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
 (lithium determination in sea water and serum by solvent extraction and spectrophotometry using octabromo tetrakis sulfonatophenyl porphyrin)
 RN 176173-80-1 CAPLUS
 CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis-, ion(4-) (9CI) (CA INDEX NAME)



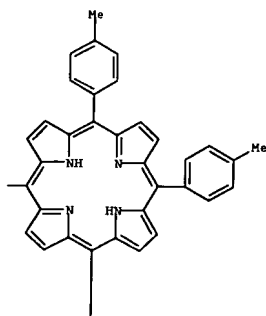
REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 63 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1999:395187 CAPLUS
 DOCUMENT NUMBER: 131:235638
 TITLE: Intramolecular Electron Transfer of Diporphyrins Comprised of Electron-Deficient Porphyrin and Electron-Rich Porphyrin with Photocontrolled Isomerization. [Erratum to document cited in CA130:160405]
 AUTHOR(S): Tsuchiya, Shinji
 CORPORATE SOURCE: Institute Industrial Science, Univ. Tokyo, Tokyo, 106, Japan
 SOURCE: Journal of the American Chemical Society (1999), 121(27), 6521
 CODEN: JACSAT; ISSN: 0002-7863
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Reference 40 and 41 relevant to the work reported on page 53 are given.
 IT 220213-35-4
 RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); FORM (Formation, nonpreparative); PROC (Process)
 (fluorescence and photoisomerization and photoinduced intramol. electron-transfer of azobenzene-linked diporphyrin Zn complexes and free base analogs (Erratum))
 RN 220213-35-4 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15-tris(4-methylphenyl)-20-[4-[(1Z)-[4-[10,15,20-tris(4-methylphenyl)-21H,23H-porphin-5-yl]phenyl]azo]phenyl]- (9CI) (CA INDEX NAME)
 Double bond geometry as shown.

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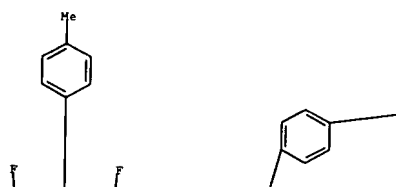


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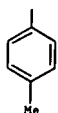
L6 ANSWER 63 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15-tris(4-methylphenyl)-20-[4-[(1E)-[4-[10,15,20-tris(4-methylphenyl)-21H,23H-porphin-5-yl]phenyl]azo]phenyl]- (9CI) (CA INDEX NAME)
 Double bond geometry as shown.

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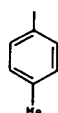


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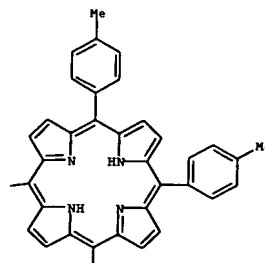
PAGE 2-A

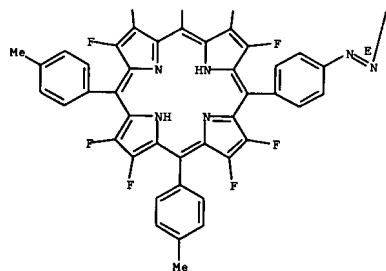


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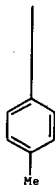


IT 220213-34-3P
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
 (fluorescence and photoisomerization and photoinduced intramol. electron-transfer of azobenzene-linked diporphyrin Zn complexes and free base analogs (Erratum))
 RN 220213-34-3 CAPLUS





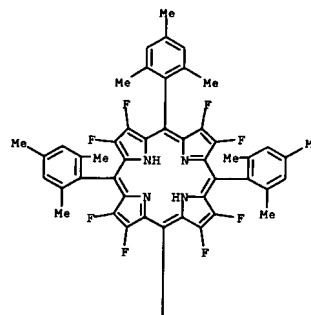
PAGE 2-A



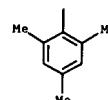
PAGE 2-B

IT 220213-36-5
 RL: FRP (Properties)
 (fluorescence quenching by electron transfer from electron-rich to
 electron-deficient porphyrin in relation to photophysics of
 azobenzene-linked diporphyrins (Erratum))
 RN 220213-36-5 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(2,4,6-
 trimethylphenyl)- (9CI) (CA INDEX NAME)

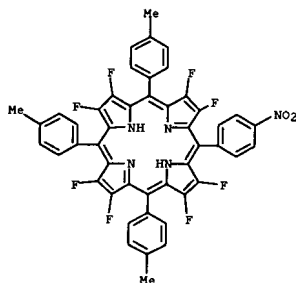
PAGE 1-A



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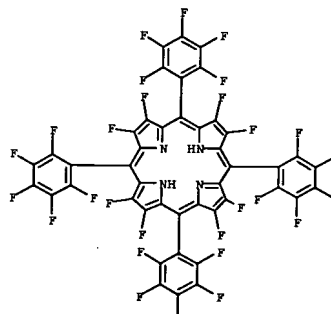


IT 220213-37-6
 RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
 (in synthesis of azobenzene-linked diporphyrin Zn complexes (Erratum))
 RN 220213-37-6 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15-tris(4-
 methylphenyl)-20-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



L6 ANSWER 64 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1999:269042 CAPLUS
 DOCUMENT NUMBER: 130:304300
 TITLE: 2,3,7,8,12,13,17,18-Octafluoro-5,10,15,20-
 tetrakis(pentafluorophenyl)porphyrin
 AUTHOR(S): Leroy, Jacques; Bondon, Arnaud; Toupet, Loic
 CORPORATE SOURCE: Ecole Normale Supérieure, Dep. Chim., URA CNRS, Paris,
 75231, Fr.
 SOURCE: Acta Crystallographica, Section C: Crystal Structure
 Communications (1999), C55(3), 464-466
 CODEN: ACSCEE; ISSN: 0108-2701
 PUBLISHER: Munksgaard International Publishers Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The core of the title compound, C44H2F28N4, is essentially planar while the
 pentafluorophenyl groups are nearly perpendicular to the mean porphyrin
 plane. The mol. is centrosym. Crystallog. data are given.
 IT 121399-88-0
 RL: FRP (Properties)
 (crystal structure of)
 RN 121399-88-0 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-
 tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

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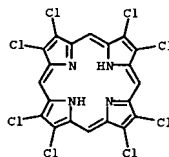
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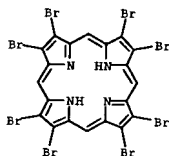
13

THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

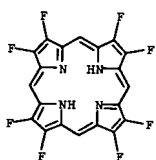
L6 ANSWER 65 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1999:260115 CAPLUS
 DOCUMENT NUMBER: 131:129798
 TITLE: Effects of halogenation on the ionized and excited states of free-base and zinc porphyrins
 AUTHOR(S): Nguyen, Kiet A.; Day, Paul N.; Pachter, Ruth
 CORPORATE SOURCE: Air Force Research Laboratory, AFRL/MLPV, Materials and Manufacturing Directorate, Wright-Patterson Air Force Base, OH, 45433-7702, USA
 SOURCE: Journal of Chemical Physics (1999), 110(18), 9135-9144
 CODEN: JCPSA6; ISSN: 0021-9606
 PUBLISHER: American Institute of Physics
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Ab initio electronic structure theory has been applied to study the effects of β -halogenation on the structure, ionization potentials (IP), and electronic spectra of free-base (PH2) and zinc porphyrins (ZnP). Electronic and IR (IR) spectra of β -octahalogenated free-base (β -PX₈H₂; X=F, Cl, Br) and zinc porphyrins (β -ZnPX₈; X=F, Cl, Br) are predicted using TDDFT, B3LYP, and CIS methods. Computations of the excitation energies and IPs are also carried out using structures obtained with the B3LYP d. functional. Valence IPs of PH₂ and ZnP increase significantly upon β -halogenation. Except for the fluoro group, all β -halogen auxochromes slightly red shift the UV and visible bands of the free-base and zinc porphyrin chromophores. β -Halogenation significantly red shifts the B bands with increasing magnitude upon going down the period. In addition, we gauge the effects of β -halogenation on the thermodyn. stability of ZnP by calculating the metal binding energies for β -ZnPX₈. The authors found that all β -ZnPX₈ have lower metal binding energies than the corresponding binding energy predicted for ZnP. The metal binding energies for zinc porphyrins are significantly larger (.apprx.2 eV) than the H₂ elimination enthalpies of the corresponding free-base analogs.
 IT 144811-81-4, Octachloroporphine 144811-83-6, Octafluoroporphine
 RL: PRP (Properties)
 (effects of halogenation on the ionized and excited states of free-base and zinc porphyrins)
 RN 144811-81-4 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro- (9CI) (CA INDEX NAME)



RN 144811-83-6 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo- (9CI) (CA INDEX NAME)

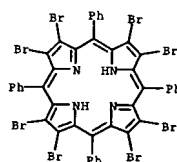


RN 144811-86-9 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro- (9CI) (CA INDEX NAME)

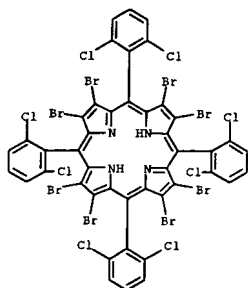


REFERENCE COUNT: 95 THERE ARE 95 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 66 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1999:83211 CAPLUS
 DOCUMENT NUMBER: 130:204223
 TITLE: Synthesis and characterization of porphyrin complexes of iron(III) and manganese(III)
 AUTHOR(S): Krishna, V.; Agarwal, D. D.; Bayrappa, G.; Rastogi, Rachana
 CORPORATE SOURCE: Dept. of IPC, Indian Institute of Science, Bangalore, 560 012, India
 SOURCE: Indian Journal of Chemistry, Section A: Inorganic, Bio-inorganic, Physical, Theoretical & Analytical Chemistry (1998), 37A(10), 918-920
 CODEN: ICACRC; ISSN: 0376-4710
 PUBLISHER: National Institute of Science Communication, CSIR
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The porphyrin complexes of Fe(III) and Mn(III) bearing electron withdrawing substituents at β -pyrrole carbons exhibit interesting electronic structure. Porphyrin ligands studied include 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-21H,23H-porphyrin and the 5,10,15,20-tetrakis(2,6-dichlorophenyl) derivative. The complexes are electroactive and show reversible redox behavior. Coulometric data suggest that oxidation and reduction involves one-electron transfer each.
 IT 131214-86-3
 RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent) (complexation with iron(III) and manganese(III), and redox potentials of)
 RN 131214-86-3 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

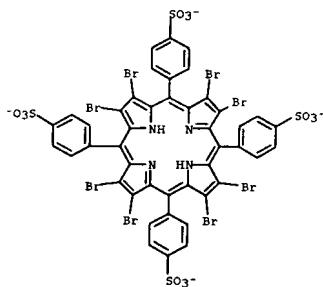


IT 107035-95-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and complexation with iron(III) and manganese(III))
 RN 107035-95-0 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,6-dichlorophenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

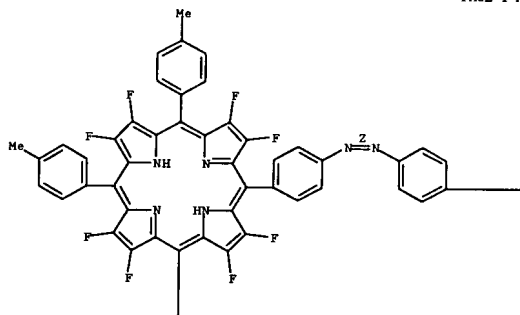
L6 ANSWER 67 OF 148 CAPLUS COPYRIGHT 2005 ACS ON STN
 ACCESSION NUMBER: 1999:19120 CAPLUS
 DOCUMENT NUMBER: 130:162452
 TITLE: Trace analysis of lithium with a water-soluble porphyrin
 AUTHOR(S): Tabata, Masaaki; Sun, Haiping; Nishimoto, Jun
 CORPORATE SOURCE: Department of Chemistry, Faculty of Science and Engineering, Saga University, Saga, 840-8502, Japan
 SOURCE: Journal of Inclusion Phenomena and Molecular Recognition in Chemistry (1998), 32(2-3), 267-281
 CODEN: JIMCEN; ISSN: 0923-0750
 PUBLISHER: Kluwer Academic Publishers
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A water-soluble porphyrin (2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(4-sulfonatophenyl)porphyrin; H2 obtpps4-; H2P4-) was synthesized and developed for the determination and separation of Li ion in aqueous solution. The octabromo groups lower the basicity of the porphyrin by their electron-withdrawing effect, and enable the porphyrin to react with Li ion in alkaline aqueous solution to form the Li complex along with a shift of absorption maxima: λ_{max} (log ϵ /mol⁻¹ dm³ cm⁻¹) of the Li porphyrin are 490.5 nm (5.31) and 734 nm (4.36). Na and K ions did not react with the porphyrin. The equilibrium constant for the reaction $Li^+ + HP5^- \rightleftharpoons [LiP]5^-$ is 104.21. The [LiP]5⁻ can be extracted into CHCl₃ as an ion-pair complex with Bu₄N ion (X⁺) and the extracted X5LiP dissoc. to X4LiP⁻ and X⁺ in CHCl₃. The extraction constant for the reaction of [LiP5⁻]_a + 5[X⁺]_a \rightleftharpoons [X4LiP⁻]_o + [X⁺]_o is (8.4 ± 0.7) + 1012 mol⁻⁴ dm¹², where subscripts of a and o denote chemical species in aqueous and organic phases, resp. The above results were developed for the determination of Li in serum, sea water and hot spring H₂O samples at 0.07-0.7 mg dm⁻³ (1 + 10⁻⁵ - 1 + 10⁻⁴ mol dm⁻³). The interference of heavy metal ions was masked by N,N'-1,2-ethanediylbis[N-(carboxymethyl)glycinato]magnesium(II) ((Mg(EDTA))₂-) or H₄EDTA if sample contain Mg(II) ion.
 IT 176173-80-1F, 2,3,7,8,12,13,17,18-Octabromo-5,10,15,20-tetrakis(4-sulfonatophenyl)porphyrin
 RL: ARG (Analytical reagent use); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses) (trace determination of lithium with a water-soluble porphyrin by extraction-spectrophotometry)
 RN 176173-80-1 CAPLUS
 CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis-, ion(4-) (9CI) (CA INDEX NAME)



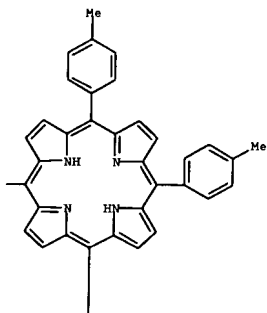
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 68 OF 148 CAPLUS COPYRIGHT 2005 ACS ON STN
 ACCESSION NUMBER: 1998:807525 CAPLUS
 DOCUMENT NUMBER: 130:160405
 TITLE: Intramolecular Electron Transfer of Diporphyrins Comprised of Electron-Deficient Porphyrin and Electron-Rich Porphyrin with Photocontrolled Isomerization
 AUTHOR(S): Tsuchiya, Shinji
 CORPORATE SOURCE: Institute of Industrial Science, University of Tokyo, Minato-Ku Tokyo, 106, Japan
 SOURCE: Journal of the American Chemical Society (1999), 121(1), 48-53
 CODEN: JACSAT; ISSN: 0002-7863
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB New azobenzene-linked diporphyrin Zn complexes and free base analogs were synthesized in an attempt to develop new materials for mol. electronics. These diporphyrin Zn complexes and the corresponding diporphyrins consist of electron-deficient porphyrin Zn complex and electron-rich porphyrin Zn complex or electron-deficient porphyrin and electron-rich porphyrin. These compds., which are a new family of diporphyrins, exhibited the photoresponsive property with a structural change in the antenna; the trans-cis photoisomerization and cis-trans thermal recovery occurred and this process was reversible. A particularly noteworthy characteristic of the diporphyrin Zn complex is that its fluorescence spectrum changes with isomerization; the fluorescence intensity of the cis-isomer produced by photoirradn. is smaller than that of the trans-isomer. This fluorescence quenching of the cis-isomer arises from the intramol. electron transfer from electron-rich porphyrin Zn complex to electron-deficient porphyrin Zn complex. Similar phenomena were observed for azobenzene-linked diporphyrins. This discovery that intramol. electron transfer between the porphyrin rings is caused by photocontrolled isomerization is worthy of notice. Adnl., these compds. bearing eight fluorine atoms at the 8-position of one porphyrin ring are the ideal materials for the practical application, because of their robust properties. This finding clearly suggests that new mol. are particularly useful in the development of photocontrolled mol. electronics such as mol. switches.
 IT 220213-35-4
 RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); FORM (Formation, nonpreparative); PROC (Process) (fluorescence and photoisomerization and photoinduced intramol. electron-transfer of azobenzene-linked diporphyrin Zn complexes and free base analogs)
 RN 220213-35-4 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15-tris(4-methylphenyl)-20-[(12)-[4-(10,15,20-tris(4-methylphenyl)-21H,23H-porphin-5-yl)phenyl]azo]phenyl]- (9CI) (CA INDEX NAME)
 Double bond geometry as shown.

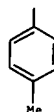
PAGE 1-A



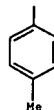
PAGE 1-B



PAGE 2-A

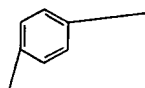
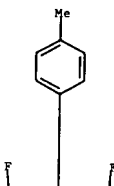


PAGE 2-B

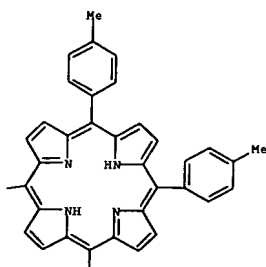


IT 220213-34-3P
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
 (fluorescence and photoisomerization and photoinduced intramol. electron-transfer of azobenzene-linked diporphyrin Zn complexes and free base analogs)
 RN 220213-34-3 CAPLUS
 CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15-tris(4-methylphenyl)-20-[4-[(1E)-[4-[[10,15,20-tris(4-methylphenyl)-21H,23H-porphin-5-yl]phenyl]azo]phenyl]]- (9CI) (CA INDEX NAME)
 Double bond geometry as shown.

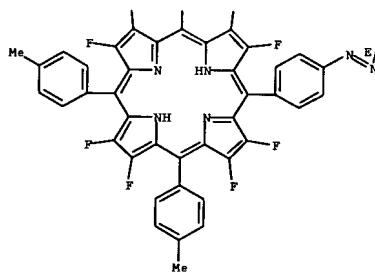
PAGE 1-A



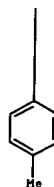
PAGE 1-B



PAGE 2-A

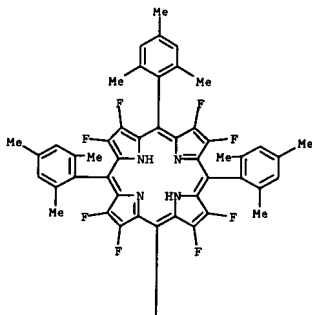


PAGE 2-B

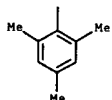


IT 220213-36-5
 RL: PRP (Properties)
 (fluorescence quenching by electron transfer from electron-rich to electron-deficient porphyrin in relation to photophysics of azobenzene-linked diporphyrins)
 RN 220213-36-5 CAPLUS
 CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

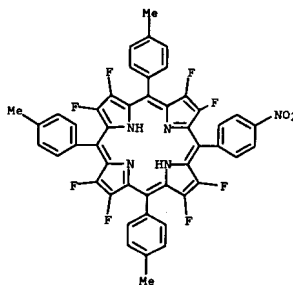
PAGE 1-A



PAGE 2-A



IT 220213-37-6
 RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
 (in synthesis of azobenzene-linked diporphyrin Zn complexes)
 RN 220213-37-6 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15-tris(4-methylphenyl)-20-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

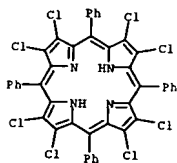


REFERENCE COUNT: 72 THERE ARE 72 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

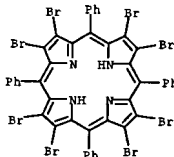
L6 ANSWER 69 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1998:805861 CAPLUS
 DOCUMENT NUMBER: 130:188901
 TITLE: Structure-optical property relationships of porphyrins
 AUTHOR(S): Su, Weijie; Cooper, Thomas M.; Nguyen, Kiet; Brant, Mark C.; Brandelik, Donna; McLean, Daniel G.
 CORPORATE SOURCE: Wright Laboratory, WL/MLPJ, Wright-Patterson AFB, OH, 45433, USA
 SOURCE: Proceedings of SPIE-The International Society for Optical Engineering (1998), 3472(Nonlinear Optical Liquids for Power Limiting and Imaging), 136-143
 CODEN: PSISDG; ISSN: 0277-786X
 PUBLISHER: SPIE-The International Society for Optical Engineering
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Porphyrins are attractive compds. for optical applications. The authors were studying the relation between mol. structure and optical properties of a number of porphyrin compds. Structural variations explored include insertion of metal ions, extension of conjugation, halogenation and alkylation either at the pyrrole position or the meso-aryl groups. The characterization of these chromophores includes measurement of UV/visible, fluorescence and fluorescence lifetimes. Also, the authors have studied their nonlinear absorption, excitation dynamics. The significant factors influencing limiting behavior appear to be the heavy atom effect, electron donating and withdrawing substituents conformation distortion and changes in conjugation. Detailed understanding will be gained from measurements of photophys. parameters underlying limiting behavior.

IT 120644-25-9 131214-86-3
 RL: FRP (Properties)
 (structure-optical property relationships of porphyrins)
 RN 120644-25-9 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



RN 131214-86-3 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

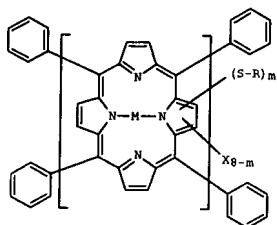
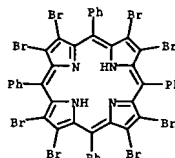


REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 70 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1998:795635 CAPLUS
 DOCUMENT NUMBER: 130:102947
 TITLE: Porphyrin compound and laser-recordable optical recording medium using it
 INVENTOR(S): Masaoka, Toshihiro; Terao, Hiroshi; Kumagaya, Youjiro; Tsukahara, Hiroshi; Misawa, Tsutayoshi; Takuma, Keisuke
 PATENT ASSIGNEE(S): Mitsui Chemicals Inc., Japan; Yamamoto Chemicals Inc.
 SOURCE: Jpn. Kokai Tokkyo Koho, 17 pp.
 CODEN: JKOXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10330632	A2	19981215	JP 1997-138509	19970528
PRIORITY APPLN. INFO.:			JP 1997-138509	19970528
OTHER SOURCE(S):				
GI				

L6 ANSWER 70 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

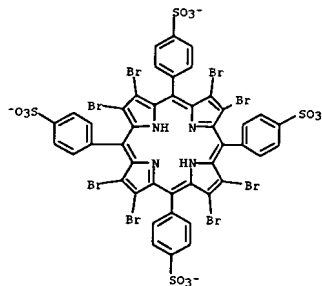


AB The porphyrin compound comprises I [R = alkyl, (un)substituted Ph, naphthyl; X = H, halo; m = 1-8; M = 2H, divalent metal, trivalent or tetravalent metal derivative]. The recording medium has a recording layer containing
 I. The medium showed high sensitivity for 520-690-nm laser light.
 IT 131214-86-3, 2,3,7,8,12,13,17,18-Octabromo-5,10,15,20-tetraphenylporphyrin
 RL: RCT (Reactant); RACT (Reactant or reagent) (thioetherified porphyrin compound for laser-recordable optical recording medium)
 RN 131214-86-3 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

L6 ANSWER 71 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1998:593286 CAPLUS
 DOCUMENT NUMBER: 129:266109
 TITLE: Kinetics and mechanism of the reaction of mercury(II) with a water-soluble octabromoporphyrin
 AUTHOR(S): Nahar, N.; Tabata, M.
 CORPORATE SOURCE: Department of Chemistry, Faculty of Science and Engineering, Saga University, Saga, 840, Japan
 SOURCE: Journal of Porphyrins and Phthalocyanines (1998), 2(4-5), 397-403
 CODEN: JPPHFZ; ISSN: 1088-4246
 PUBLISHER: John Wiley & Sons Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The reaction of mercury(II) hydroxide with 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(4-sulfonatophenyl)porphyrin, (TPPSBr8)H24- (H2P4-), to form the mercury(II) porphyrin [(TPPSBr8)Hg]4- (HgP4-) was investigated in the pH range 6.2-8.5. The observed rate constant was first-order with respect to the mercury(II) concentration and decreased with increasing pH from pH 6.2 to 7.5 and then increased from pH 7.5 to 8.5. The rate expression was written as $d[\text{HgP4-}]/dt = (KHPK_1[\text{H}^+])^{-1} + KHPK_1[\text{H}^+]) (1 + K_1[\text{H}^+] + K_1[\text{H}^+])^{-1} - 1[\text{Hg}(\text{OH})_2][\text{H}_2\text{P4-}]$. The KHP, KHP2 and KHP3 values were found to be $(1.33 \pm 0.02) + 108$, $(5.50 \pm 0.08) + 106$ and $(1.40 \pm 0.08) + 108 \text{ M}^{-1} \text{ s}^{-1}$ resp., with $K_1 = [\text{H}_3\text{P3-}]/[\text{H}_2\text{P4-}] - 1[\text{H}^+] - 1 = 104.83 \pm 0.04$ and $K_1 = [\text{H}_5\text{P5-}]/[\text{H}^+][\text{H}_2\text{P4-}] - 1 = 1010.02 \pm 0.02$. The activation parameters were $\Delta H^\ddagger_{\text{thermod.}} = 94 \pm 12 \text{ kJ mol}^{-1}$ and $\Delta S^\ddagger_{\text{thermod.}} = 226 \pm 22 \text{ J K}^{-1} \text{ mol}^{-1}$ for the KHP path, $\Delta H^\ddagger_{\text{thermod.}} = 33 \pm 4 \text{ kJ mol}^{-1}$ and $\Delta S^\ddagger_{\text{thermod.}} = -6.4 \pm 0.4 \text{ J K}^{-1} \text{ mol}^{-1}$ for the KHP2 path and $\Delta H^\ddagger_{\text{thermod.}} = 40 \pm 7 \text{ kJ mol}^{-1}$ and $\Delta S^\ddagger_{\text{thermod.}} = 44 \pm 4 \text{ J K}^{-1} \text{ mol}^{-1}$ for the KHP3 path. The kinetic results show the high reactivity of mercury(II) hydroxide towards the protonated porphyrin.
 IT 176173-80-1, 2,3,7,8,12,13,17,18-Octabromo-5,10,15,20-tetrakis(4-sulfonatophenyl)porphyrin
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent) (kinetics and mechanism of reaction of mercury(II) with water-soluble octabromoporphyrin)
 RN 176173-80-1 CAPLUS
 CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis-, ion(4-) (9CI) (CA INDEX NAME)

L6 ANSWER 71 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



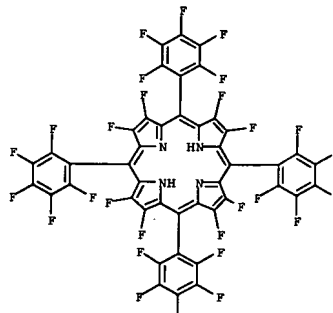
REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 72 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1998:577480 CAPLUS
DOCUMENT NUMBER: 129:253965
TITLE: 19F NMR and Structural Evidence for Spin-State
Modulation of Six-Coordinate Cobalt(II) in a Weak
Field Porphyrin Ligand
AUTHOR(S): Smirnov, Valeriy V.; Woller, Eric K.; DiMaggio, Stephen
G.
CORPORATE SOURCE: Department of Chemistry, University of
Nebraska-Lincoln, Lincoln, NE, 68588-0304, USA
SOURCE: Inorganic Chemistry (1998), 37(19), 4971-4978
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The syntheses and characterization of [2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetraphenylporphinato]cobalt, Co(F8TPP), and [2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)porphinato]cobalt, Co(F28TPP), are reported. Co(F28TPP)·2tol (tol = toluene) crystallizes in the monoclinic space group C₂h with a 22.1616(5), b 12.0274(3), c 19.9159(2) Å, β 110.645(1)°, and Z = 4 [d_{calc} = 1.818 g/cm³; μ_a(Mo Kα) = 0.50 mm⁻¹], and Co(F28TPP)·2THF crystallizes in the triclinic space group P₂1h with a 11.0691(1), b 12.0451(1), c 12.9558(2) Å, α 62.531(1), β 69.544(1), γ 76.181(1)° and Z = 1 [d_{calc} = 1.700 g/cm³; μ_a(Mo Kα) = 0.45 mm⁻¹]. A comparison of the x-ray crystal structure data from Co(F28TPP)·2tol and Co(F28TPP)·2THF indicates that the porphyrin core expands dramatically (0.08 Å) in the six-coordinate complex. Optical and 19F NMR spectroscopic studies of Co(F28TPP) in the presence of added ligand demonstrate that spin-state modulation of the six-coordinate Co(II) center is facile. Partial population of the 4E_g state is accessed upon coordination of the cobalt center with THF σ-donor ligands, while six-coordinate complexes with 1-methylimidazole result in complete conversion to the high spin state, as evinced by 280 ppm downfield chemical shifts for the β-fluorine resonances in the 19F NMR spectrum. Co(F28TPP) is the 1st example of a porphyrin which supports a high-spin cobalt ion.
IT 121399-88-0, 2,3,7,8,12,13,17,18-Octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)porphine 186885-28-9
2,3,7,8,12,13,17,18-Octafluoro-5,10,15,20-tetraphenylporphine
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of cobalt fluorinated tetraphenylporphinato complexes)
RN 121399-88-0 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

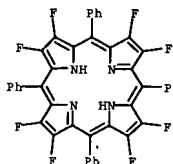
L6 ANSWER 72 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

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RN 186885-28-9 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



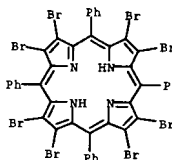
REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 73 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1998:577449 CAPLUS
DOCUMENT NUMBER: 129:269434
TITLE: Electronic, Spectral, and Electrochemical Properties
of (TPPBx)Zn Where TPPBx is the Dianion of
β-Brominated-Pyrrole Tetraphenylporphyrin and x
Varies from 0 to 8
AUTHOR(S): D'Souza, Francis; Zandler, Melvin E.; Tagliatesta,
Pietro; Ou, Zhongping; Shao, Jianguo; Van Caemelbecke,
Eric; Kadish, Karl M.
CORPORATE SOURCE: Department of Chemistry, Wichita State University,
Wichita, KS, 67260-0051, USA
SOURCE: Inorganic Chemistry (1998), 37(18), 4567-4572
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The electronic, spectral, and electrochem. characterization of (meso-tetraphenylporphyrinato)zinc(II) complexes bearing from 0 and 8 bromo substituents at the β-pyrrole positions is reported. The studied compds. are represented as (TPPBx)Zn where TPPBx is the dianion of brominated 5,10,15,20-tetraphenylporphyrin and x varies between 0 and 8. Each porphyrin undergoes four well-defined 1-electron transfer reactions to yield porphyrin x-cation radicals and dications upon oxidation and porphyrin x-anion radicals and dianions upon reduction. Half-wave potentials for the 1st reduction of (TPPBx)Zn can be described by a single linear free energy relation, and plots of E_{1/2} vs. the number of Br groups on the complex show a linear correlation with a pos. slope of 63 mV per Br group. This is not the case for the other three electron transfer processes of the compds. where plots of E_{1/2} vs. the number of Br groups show distinctly different linear correlations for derivs. with 0-4 Br groups and those with 4-8 Br groups. The effect of increasing number of Br groups on the spectral and electrochem. properties of the neutral complexes was examined over the whole series of compds., and these exptl. results are compared to results of theor. calcs. by semiempirical MO AM1 methods using configurational interactions (CI) over the four Gouterman frontier σ-orbitals. The dihedral angle containing the four porphyrin macrocycle ring nitrogens is proposed as a measure of porphyrin ring nonplanarity, and this value increases with increasing number of Br substituents on (TPPBx)Zn. Results of the AM1-CI = 4 calcs. indicate that the spectrally determined HOMO-LUMO gap, i.e., the energy corresponding to the low-energy absorption band, varies in a nonlinear fashion with increasing number of Br substituents on the macrocycle and this is due to both the electronic effect of the substituents and the macrocycle nonplanarity. The HOMO-LUMO gaps theor. calculated by AM1-CI = 4 methods thus parallel values which are exptl. obtained by electrochem. or spectroscopy. The lack of well-defined linear free energy relations for all processes except for the 1st reduction can be explained from electronic effects caused by the halogen substituents and nonplanar macrocyclic distortions induced by steric interactions among the peripheral substituents. In the case of porphyrin dication formation, the redox potentials are virtually independent of the bromo substituents.
IT 131214-86-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of zinc brominated tetraphenylporphyrinato complex)

RN 131214-86-3 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

L6 ANSWER 73 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 1998:567479 CAPLUS

DOCUMENT NUMBER: 129:269428

TITLE: Novel covalently linked porphyrin trimers with

redox-distinct properties

AUTHOR(S): Sen, Avijit; Anandhi, U.; Krishnan, V.

CORPORATE SOURCE: Chemical Biology unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, 560 012, India

SOURCE: Tetrahedron Letters (1998), 39(36), 6539-6542

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Two novel porphyrin trimers bearing different metal centers and/or different peripheral substituents were synthesized. These systems display interesting spectral and electrochem. redox properties.

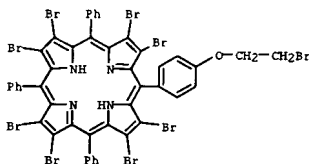
IT 213414-00-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(for preparation of ethanedioxy-linked tetraphenylporphyrin trimer)

RN 213414-00-7 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5-[4-(2-bromethoxy)phenyl]-10,15,20-triphenyl- (9CI) (CA INDEX NAME)



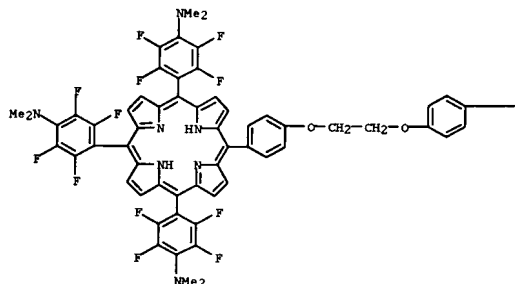
IT 213482-55-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation, cyclic voltammetry, NMR and electronic absorption spectra, and fluorescence quenching)

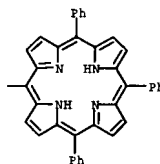
RN 213482-55-4 CAPLUS

CN Benzenamine, 4,4',4''-[20-[4-[2-[4-[C-[3,5-dimethyl-4-[2-[4-(2,3,7,8,12,13,17,18-octabromo-10,15,20-triphenyl-21H,23H-porphin-5-yl)phenoxy]ethoxy]phenyl]-10,15,20-triphenyl-21H,23H-porphin-5-yl)phenoxy]ethoxy]phenyl]-21H,23H-porphine-5,10,15-triyl]tris[2,3,5,6-tetrafluoro-N,N-dimethyl- (9CI) (CA INDEX NAME)

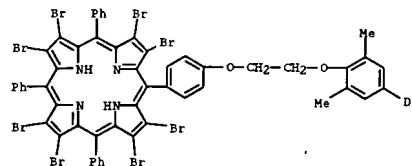
PAGE 1-A



PAGE 1-B



PAGE 2-A



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 1998:564606 CAPLUS

DOCUMENT NUMBER: 129:260548

TITLE: Novel 1,2-Rearrangement of Porphyrinatorrhodium(III) Alkyls: Cis β -Hydride Elimination/Olefin Metal-Hydride Insertion Pathway

AUTHOR(S): Mak, Kin Wah; Chan, Kin Shing

CORPORATE SOURCE: Department of Chemistry, The Chinese University of Hong Kong, Shatin, Hong Kong

SOURCE: Journal of the American Chemical Society (1998),

120(37), 9686-9687

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Rh(bocp)R (bocp = 5,10,15,20-tetrakis-(4'-tert-butylphenyl)-2,3,7,8,12,13,17,18-octachloroporphyrinate; R = CH₂CH₂C(CH₃)₂X-p; X = NO₂, Cl, H, Me, OMe) were prepared and their thermal isomerization to Rh(bocp)R' (R' = CHMeC(CH₃)₂X-p) was studied. The authors deduced a cis β -hydride elimination/olefin metal-hydride insertion pathway. The equilibrium constant and kinetics parameters, including deuterium kinetic isotope effect, were determined

IT 213481-24-4P, 5,10,15,20-Tetrakis(4-tert-butylphenyl)-

2,3,7,8,12,13,17,18-octachloroporphyrin

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

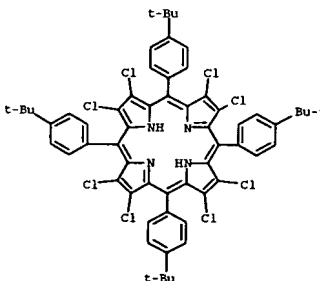
(intermediate for preparation of rhodium tetraaryloctachloroporphyrinato

phenylethyl complexes)

RN 213481-24-4 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis[4-

(1,1-dimethylethyl)phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 76 OF 148 CAPLUS COPYRIGHT 2005 ACS ON STN

ACCESSION NUMBER:

1998:466549 CAPLUS

DOCUMENT NUMBER:

129:130641

TITLE:

Spectrophotometric determination of lithium ion using a water-soluble octabromoporphyrin in aqueous solution
Tabata, M.; Nishimoto, T.; Kusano, T.
Department of Chemistry, Faculty of Science and Engineering, Saga University, Saga, 840, Japan
Talanta (1998), 46(4), 703-709
CODEN: TLNTA2; ISSN: 0039-9140
Elsevier Science B.V.

PUBLISHER:

DOCUMENT TYPE:

LANGUAGE:

English

AB A water-soluble porphyrin, (2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(4-sulfonatophenyl)porphyrin; H2obtpps⁴⁻) was synthesized and developed for the determination of Li ion in aqueous solution. The octabromo groups lower the basicity of the porphyrin by their electron-withdrawing effect, and enable the porphyrin to react with the Li ion in alkaline solution to form the Li

complex along with a shift of absorption maximum: $\lambda_{\text{maximum}}/\text{nm}$ (log $\epsilon/\text{mol}^{-1} \text{ dm}^3 \text{ cm}^{-1}$) of the Li porphyrin are 490.5 nm (5.31) and 734 nm (4.36). Na and K ions did not react with the porphyrin. The equilibrium constant for the reaction $\text{Li}^+ + \text{Hobtpps}^{5-} \rightleftharpoons \text{Li}(\text{obtpps})^{5-} + \text{H}^+$ is 10^{-8.80} and the conditional formation constant of the $[\text{Li}(\text{obtpps})]^{5-}$ at pH 13 is 104.21. The above results were applied to the determination of Li ion in

aqueous solution. The interference from transition and heavy metal ions was masked by using N,N'-1,2-ethanedithiolbis[N(carboxymethyl)glycinato]magnesium (II) ([Mg(EDTA)]²⁻) solution. Absorbance at 490 nm was measured against a blank solution. A calibration graph was linear at 0.007-0.7 $\mu\text{g cm}^{-3}$ (1 + 10⁻⁶ - 1 + 10⁻⁴ mol dm⁻³) of Li(I) with a correlation factor of 0.967. Li ion less than ppm level was determined spectrophotometrically in

aqueous solution. The proposed method was applied to the determination of Li in human

serum and sea water samples.

IT 176173-80-1P, 2,3,7,8,12,13,17,18-Octabromo-5,10,15,20-tetrakis(4-sulfonatophenyl)porphyrin

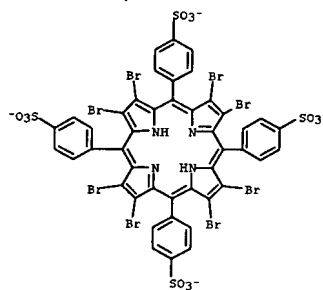
RL: ARG (Analytical reagent use); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses) (spectrophotometric determination of lithium ion using a water-soluble octabromoporphyrin in aqueous solution)

RN 176173-80-1 CAPLUS

CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis-, ion(4-) (9CI) (CA INDEX NAME)

L6 ANSWER 76 OF 148 CAPLUS COPYRIGHT 2005 ACS ON STN

(Continued)



REFERENCE COUNT:

24

THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 77 OF 148 CAPLUS COPYRIGHT 2005 ACS ON STN

ACCESSION NUMBER:

1998:401896 CAPLUS

DOCUMENT NUMBER:

129:154264

TITLE:

Fast atom bombardment mass spectral observations on some β -halogenated tetraphenylporphyrins and their iron derivatives. [Erratum to document cited in CA128:250176]

AUTHOR(S):

Boschi, Tristano; D'Arcangelo, Giuseppe; Tagliatesta, Pietro

CORPORATE SOURCE:

Dip. Scienze Tecnologie Chimiche, Università Studi Roma "Tor Vergata", Rome, I-00173, Italy

SOURCE:

European Mass Spectrometry (1998), 4(1), 83

PUBLISHER:

CODEN: EMSPPW; ISSN: 1356-1049

DOCUMENT TYPE:

IN Publications

LANGUAGE:

English

AB The captions for Figures 5, 6, and 7 and for Figures 8 and 9 were transposed in press; the correct captions are given.

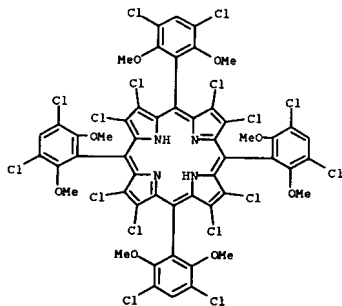
IT 180711-85-7

RL: PRP (Properties)

(fast atom bombardment mass spectral observations on β -halogenated tetraphenylporphyrins and iron derivs. (Erratum))

RN 180711-85-7 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(3,5-dichloro-2,6-dimethoxyphenyl)- (9CI) (CA INDEX NAME)



L6 ANSWER 78 OF 148 CAPLUS COPYRIGHT 2005 ACS ON STN

ACCESSION NUMBER:

1998:381712 CAPLUS

DOCUMENT NUMBER:

128:322841

TITLE:

Peroxide Decoloration of Azo Dyes Catalyzed by Polyethylene Glycol-Linked Manganese Halogenated Porphyrins

AUTHOR(S):

Nango, Mamoru; Iwasaki, Toyota; Takeuchi, Yoshito;

CORPORATE SOURCE:

Kurono, Yukihisa; Tokuda, Junko; Oura, Ritsuko
Department of Applied Chemistry, Nagoya Institute of Technology, Nagoya, 466, Japan

SOURCE:

Langmuir (1998), 14(12), 3272-3278

PUBLISHER:

CODEN: LANGD5; ISSN: 0743-7463

DOCUMENT TYPE:

American Chemical Society

LANGUAGE:

Journal

AB Polyethylene glycol (PEG)-linked manganese halogenated porphyrins (Chart 1) catalyzed oxidation of azo dyes (Chart 2) by H2O2 under mild conditions such as pH 8.0 at 25 °C especially when imidazole was present, causing the decoloration of azo dyes. The decoloration of azo dyes by synthetic manganese porphyrins under mild conditions was first reported. The decoloration rate depended on the structures of the porphyrins, in which the largest rate was observed in the presence of PEG-MnDCTP. The decoloration may be contributed by radical species rather than electrophilic species, consistent with the side-chain oxidation of toluene. Kinetics on polyethylene glycol-linked manganese porphyrin-catalyzed decoloration of C.I. Acid Orange 7 by hydrogen peroxide revealed that the decoloration was contributed at the oxidation process by manganese porphyrins

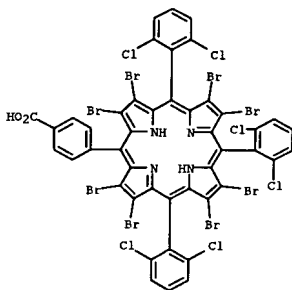
with hydrogen peroxide in the polymer domain rather than the complex-formation process between manganese porphyrins and azo dyes.

IT 206987-42-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (intermediate for catalysts; peroxide decoloration of azo dyes catalyzed by polyethylene glycol-linked manganese halogenated porphyrins)

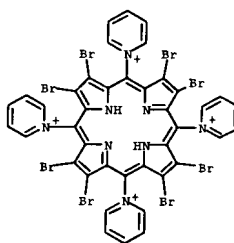
RN 206987-42-0 CAPLUS

CN Benzoic acid, 4-[2,3,7,8,12,13,17,18-octabromo-10,15,20-tris(2,6-dichlorophenyl)-21H,23H-porphin-5-yl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

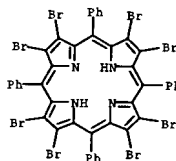
L6 ANSWER 79 OF 148 CAPLUS COPYRIGHT 2005 ACS ON STN
 ACCESSION NUMBER: 1998:336754 CAPLUS
 DOCUMENT NUMBER: 129:67628
 TITLE: Ab initio calculations on porphyrins in the condensed phase
 AUTHOR(S): Day, P. N.; Wang, Z.; Pachter, R.
 CORPORATE SOURCE: Materials Directorate, Air Force Research Laboratory, Wright-Patterson AFB, OH, 45433, USA
 SOURCE: Materials Research Society Symposium Proceedings (1998), 488(Electrical, Optical, and Magnetic Properties of Organic Solid-State Materials IV), 853-858
 CODEN: MRSPDH; ISSN: 0272-9172
 PUBLISHER: Materials Research Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Porphyrins are a promising class of materials for optical limiting applications, and in the condensed phase solvent effects have been shown to be significant. The authors report results with a method designed to simulate the effects of discrete solvent mols., namely the effective fragment potential (EFP) approach which has been implemented for use in ab initio calcs. Further, a simulated annealing (SA) method has been implemented with the EFP solvation model in an attempt to solve the problem of multiple min. in clusters of mols. The results with this method indicate some success on models of aqueous formamide and aqueous glutamic acid. Ab initio calcs. can now be carried out on porphyrins, and the solvation methods are being updated for their use on these systems.
 IT 208995-40-8
 RL: PRP (Properties) (ab initio calcs. on octabromotetrapyrrolineporphyrin cation in the condensed phase)
 RN 208995-40-8 CAPLUS
 CN Pyridinium, 1,1',1'',1'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 80 OF 148 CAPLUS COPYRIGHT 2005 ACS ON STN
 ACCESSION NUMBER: 1998:302287 CAPLUS
 DOCUMENT NUMBER: 129:59211
 TITLE: Saddle-shaped dioxo-ruthenium(VI) and -osmium(VI) 2,3,5,7,8,10,12,13,15,17,18,20-dodecaphenylporphyrin (H2dpp) complexes. Synthesis, spectral characterization and alkene oxidation by [RuVI(dpp)O2]
 AUTHOR(S): Liu, Chun-Jing; Yu, Wing-Yiu; Peng, Shie-Ming; Mak, Thomas C. W.; Che, Chi-Ming
 CORPORATE SOURCE: Department of Chemistry, The University of Hong Kong, Hong Kong
 SOURCE: Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1998), (11), 1805-1812
 CODEN: JCDTBI; ISSN: 0300-9246
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English

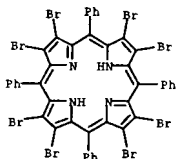
L6 ANSWER 80 OF 148 CAPLUS COPYRIGHT 2005 ACS ON STN (Continued)



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

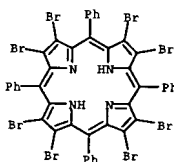
AB An improved procedure for the preparation of the saddle-distorted porphyrin 2,3,5,7,8,10,12,13,15,17,18,20-dodecaphenylporphyrin (H2dpp) (yield = 75%) based on the Suzuki cross-coupling reaction between phenylboronic acid PhB(OH)2 and [2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenylporphyrin] has been developed. X-Ray diffraction studies of [MII(dpp)(CO)(py)] (M = Ru 1 or Os 3) showed that 1 and 3 are isostructural, and the porphyrin macrocycles exhibit severe out-of-plane saddle and ruffle distortions. In both 1 and 3 the pyrrole rings are alternately tilted up and down with respect to the least-squares plane of the 25-atom porphyrin core, and the pyrrole carbons experience an average displacement of 0.769 Å from the least-squares plane compared to 0.78 Å for free H2dpp, whereas the Ru and Os atoms are displaced by 0.1006 and 0.0792 Å from the 25-atom porphyrin core resp. The complex [RuVI(dpp)O2] 2, prepared by m-chloroperoxybenzoic acid oxidation, is an active oxidant for alkene epoxidns. In CH2Cl2 [containing 2% (weight/weight) pyrazole], styrene, norbornene and cis-stilbene were oxidized selectively to their resp. epoxides in excellent yield. Complete stereoretention was observed for the oxidation of cis-stilbene, however oxidation of cis-β-methylstyrene afforded significant amts. of trans-epoxide suggesting that a carbocationic mechanism is operative. The crystal structure of the complex [RuIV(dpp)(pz)2] (5), the product of the stoichiometric alkene oxidns., was determined. Magnetic susceptibility measurement (μeff = 3.24 μB) suggests the formulation of RuIV with two unpaired electrons in its electronic ground state. The Ru-N (pz) bond distances are 2.022 (13) and 2.083 (12) Å. The reactions of 2 with alkenes in CH2Cl2 (with 2% Hpz) follow second-order kinetics: rate = k1[2][alkene]. For norbornene and styrene, the second-order rate consts., k1, in CH2Cl2 at 25.9 °C are (3.79 ± 0.04) × 10⁻³ and (4.78 ± 0.09) × 10⁻³ dm³ mol⁻¹ s⁻¹ resp.
 IT 131214-86-3, [2,3,7,8,12,13,17,18-Octabromo-5,10,15,20-tetraphenylporphyrin]
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (saddle-shaped dioxo-ruthenium(VI) and -osmium(VI) 2,3,5,7,8,10,12,13,15,17,18,20-dodecaphenylporphyrin (H2dpp) complexes and synthesis, spectral characterization and alkene oxidation by [RuVI(dpp)O2])
 RN 131214-86-3 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

L6 ANSWER 81 OF 148 CAPLUS COPYRIGHT 2005 ACS ON STN
 ACCESSION NUMBER: 1998:269879 CAPLUS
 DOCUMENT NUMBER: 128:328423
 TITLE: Investigation of Reverse-Saturable Absorption in Brominated Porphyrins
 AUTHOR(S): Su, Weijie; Cooper, Thomas M.; Brant, Mark C.
 CORPORATE SOURCE: Air Force Research Laboratory AFRL/MLPJ, Wright-Patterson Air Force Base, Dayton, OH, 45433, USA
 SOURCE: Chemistry of Materials (1998), 10(5), 1212-1213
 CODEN: CMATEX; ISSN: 0897-4756
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Nonlinear absorption data are given for both octabromotetraphenylporphyrin (H2OBP) and some metallooctabromotetraphenylporphyrins (MOBP). ZnOBP had strong nonlinear absorption comparable to state-of-the-art phthalocyanine dyes.
 IT 131214-86-3
 RL: PRP (Properties)
 (reverse-saturable absorption in)
 RN 131214-86-3 CAPLUS
 CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (SCI) (CA INDEX NAME)



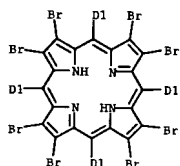
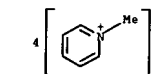
REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 82 OF 148 CAPLUS COPYRIGHT 2005 ACS ON STN
 ACCESSION NUMBER: 1998:250205 CAPLUS
 DOCUMENT NUMBER: 128:316734
 TITLE: Application of matrix-assisted laser desorption/ionization Fourier transform mass spectrometry to the analysis of planar porphyrins and highly substituted nonplanar porphyrins
 AUTHOR(S): Green, M. Kirk; Medforth, Craig J.; Muzzi, Cinzia M.; Murco, Daniel J.; Shea, Kalyan M.; Smith, Kevin M.; Lebrilla, Carlito B.; Sheinert, John A.
 CORPORATE SOURCE: Department of Chemistry, University of California at Davis, Davis, CA, 95616, USA
 SOURCE: European Mass Spectrometry (1997), 3(6), 439-451
 CODEN: EMSPPW; ISSN: 1356-1049
 PUBLISHER: IM Publications
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The applicability of matrix-assisted laser desorption/ionization (MALDI) Fourier transform mass spectrometry to the anal. of porphyrins was examined. High resolution spectra were readily obtained with good sensitivity and a detection limit ≥ 2 fmol. A mixed solvent system of toluene and ethanol (1:1 by volume) proved to be compatible with the 2,5-dihydroxybenzoic acid (DHB) matrix and solubilized most of the porphyrins examined. Porphyrins which were insol. in this solvent mixture could be dissolved in an appropriate solvent and deposited on a layer of DHB (layered MALDI). The parent ion was generally the largest peak in the spectrum, although for some metalloporphyrins the peak corresponding to (M - metal + 3H)⁺ was dominant. The extent of demetalation depends on factors such as sample preparation, the metal ion and the laser intensity. Addition of more than one hydrogen occurred in many cases but was a minor process. Spectra of compds. ionized by different methods showed increasing fragmentation in the order MALDI < layered MALDI < fast-atom bombardment < laser desorption.
 IT 131214-86-3 206349-60-2
 RL: ANT (Analyte); PRP (Properties); ANST (Analytical study)
 (MALDI Fourier transform mass spectrometry in anal. of planar porphyrins and highly substituted nonplanar porphyrins and their metal complexes)
 RN 131214-86-3 CAPLUS
 CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (SCI) (CA INDEX NAME)

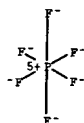


RN 206349-60-2 CAPLUS
 CN Pyridinium, (2,3,7,8,12,13,17,18-octabromo-21H, 23H-porphine-5,10,15,20-tetrayl)-tetrakis[1-methyl-, tetrakis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

L6 ANSWER 82 OF 148 CAPLUS COPYRIGHT 2005 ACS ON STN (Continued)
 CM 1
 CRN 206349-59-9
 CMF C44 H30 Br8 N8
 CCI IDS

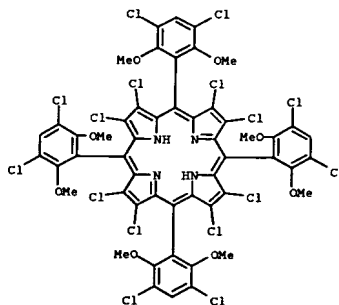


CM 2
 CRN 16919-18-9
 CMF F6 P
 CCI CCS



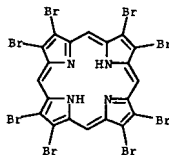
REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 83 OF 148 CAPLUS COPYRIGHT 2005 ACS ON STN
 ACCESSION NUMBER: 1998:131988 CAPLUS
 DOCUMENT NUMBER: 128:250176
 TITLE: Fast atom bombardment mass spectral observations on some β -halogenated tetraphenylphosphorins and their iron derivatives
 AUTHOR(S): Boschi, Tristano; D'Arcangelo, Giuseppe; Tagliatesta, Pietro
 CORPORATE SOURCE: Dip. Scienze Tecnologie Chimiche, Universita Studi Roma "Tor Vergata", Rome, I-00173, Italy
 SOURCE: European Mass Spectrometry (1997), 3(5), 355-360
 CODEN: EMSPPW; ISSN: 1356-1049
 PUBLISHER: IM Publications
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The fast atom bombardment mass spectral observations on some β -halogenated tetraphenylporphyrins and their iron derivs. were compared in order to investigate the relative stability of these complexes. The investigated compds. are represented as O[FeBr4TPP]2, O[FeTPP]2, O[FeTPP(4-Br)]2, O[FeTPP(4-OCH3)]2, H2(Br4TPP), Fe(Br4TPP)Cl, H2(Cl16TDCMPP) and Fe(Cl16TDCMPP)Cl where Br4TPP is the dianion of 7,8,17,18-tetrabromo-5,10,15,20-tetraphenylphosphyrin, TPP is the dianion of 5,10,15,20-tetraphenylporphyrin, TPP(4-Br) is the dianion of 5,10,15,20-tetra(4-bromo)phenylporphyrin, TPP(4-OCH3) is the dianion of 5,10,15,20-tetra(4-methoxy)phenylporphyrin and Cl16TDCMPP is the dianion of 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetra(2,6-dimethoxy-3,5-dichloro)phenylporphyrin. The stability of each mol. ion and the subsequent fragmentations were correlated to the substitution of the porphyrin rings and to the loss of steric hindrance.
 IT 180711-85-7
 RL: PRP (Properties)
 (fast atom bombardment mass spectral observations on β -halogenated tetraphenylphosphorins and iron derivs.)
 RN 180711-85-7 CAPLUS
 CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(3,5-dichloro-2,6-dimethoxyphenyl)- (9CI) (CA INDEX NAME)



L6 ANSWER 83 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

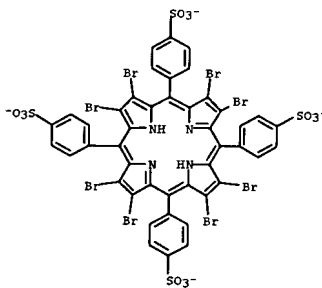
L6 ANSWER 84 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1998:99309 CAPLUS
DOCUMENT NUMBER: 128:132114
TITLE: Lithium(II) porphyrin complex for the spectrophotometric determination of lithium ion in aqueous solution
AUTHOR(S): Tabata, Masaaki; Kusano, Tohru; Nishimoto, Jun
CORPORATE SOURCE: Department of Chemistry, Faculty of Science and Engineering, Saga University, Saga, 840, Japan
SOURCE: Analytical Sciences (1997), 13(Suppl., Asianalysis IV), 157-160
CODEN: ANSCEN; ISSN: 0910-6340
PUBLISHER: Japan Society for Analytical Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A water-soluble octabromoporphyrin was synthesized for the determination of Li in water. The porphyrin reacts with Li in alkaline solution to form the Li complex along with a shift of absorption maximum to shorter wave length. Na and K ions do not react with the porphyrin. The equilibrium constant of the Li(II) porphyrin complex was determined and applied to the determination of Li in natural water. Interference of metal ions was removed by ligand buffer of Mg-EDTA complex.
IT 144811-83-6
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(lithium porphyrin complex for spectrophotometric determination of lithium in water)
RN 144811-83-6 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo- (9CI) (CA INDEX NAME)



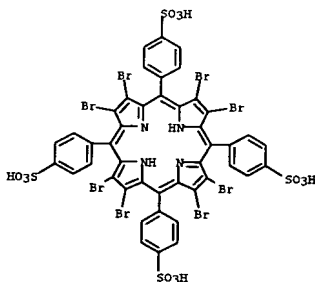
REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 85 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1998:99297 CAPLUS
DOCUMENT NUMBER: 128:249140
TITLE: Ion-pair extraction of lithium ion by a water-soluble porphyrin
AUTHOR(S): Haiping, Sun; Nishimoto, Jun; Tabata, Masaaki
CORPORATE SOURCE: Department of Chemistry, Faculty of Science and Engineering, Saga University, Saga, 840, Japan
SOURCE: Analytical Sciences (1997), 13(Suppl., Asianalysis IV), 119-122
CODEN: ANSCEN; ISSN: 0910-6340
PUBLISHER: Japan Society for Analytical Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The equilibrium of ion-pair extraction of lithium porphyrin [octabromoporphyrin: 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(4-sulfonatophenyl)porphyrin, H2obtpps4-; H2P4-] with tetrabutylammonium ion (X+) was studied at 25° and I = 0.1 (NaCl, NaOH). Extraction and dissociation consts. of the ion-pair complexes of free base porphyrin, deprotonated porphyrin and lithium porphyrin, defined as $K_{ex}(H2P) = [X4H2P]o/[H2P4-]a[X+]a4$, $K'_{ex}(HP) = [X5HP]o/[HP5-]a[X+]a5$, $K''_{ex}(LiP) = [X5LiP]o/[LiP5-]a[X+]a5$, $K_{disl}(H2P) = [X3H2P]o/[X+]o/[X4H2P]o$ and $K'_{disl}(LiP) = [X4LiP]o/[X+]o/[X5LiP]o$, were determined. These values were found to be $K_{ex}(H2P) = (9.5 \pm 1.5) + 1013$ (mol-4dm12), $K_{disl}(H2P) = (3.5 \pm 0.7) + 10-7$ (mol dm-3), $K'_{ex}(HP) = (4.7 \pm 0.4) + 1016$ (mol-5dm15) and $K''_{ex}(LiP)K'_{disl}(LiP) = (8.4 \pm 0.7) + 1012$ (mol-4dm12), resp.
IT 154783-99-0D, lithium tetrabutylammonium salts 176173-80-1
RL: NUU (Other use, unclassified); PEP (Physical, engineering or chemical process); PROC (Process); USES (Uses)
(ion-pair extraction of lithium ion by water-soluble porphyrin)
RN 154783-99-0 CAPLUS
CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis- (9CI) (CA INDEX NAME)

L6 ANSWER 85 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis-, ion(4-) (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT



RN 176173-80-1 CAPLUS

L6 ANSWER 86 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1998:33809 CAPLUS
 DOCUMENT NUMBER: 128:167041
 TITLE: DFT study of alkynylporphyrin dimers and brominated tetraphenylporphyrins
 AUTHOR(S): Wang, Zhiqiang; Day, Paul; Pachter, Ruth; Mclean, Daniel G.
 CORPORATE SOURCE: Materials Directorate, Wright Laboratory, WL/MLPJ Wright-Patterson Air Force Base, OH, 45433-7702, USA
 SOURCE: Materials Research Society Symposium Proceedings (1997), 479 (Materials for Optical Limiting II), 331-336
 CODEN: MRSPPH; ISSN: 0272-9172
 PUBLISHER: Materials Research Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

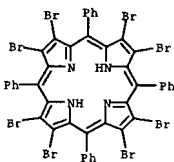
AB Geometry optimizations and electronic structure calcs. using D. Functional Theory (DFT) are reported for tetraacetyleneporphyrins (TAP), their dimers, and octabromotetraphenylporphyrins (OBP). The acetylene group contributes to the β -electron conjugation along the porphyrin ring for the HOMO and LUMO, and reduces significantly the HOMO-LUMO gap. The gap is further reduced in dimers. The planar geometry of the TAP dimer has a lower energy than the non-planar one. The geometry of HZOEP is found to be non-planar, and the distortion of porphyrin ring is shown to be closely related to the HOMO-LUMO gap.

IT 131214-86-3

RL: PRP (Properties)
 (DFT study of alkynylporphyrin dimers and brominated tetraphenylporphyrins)

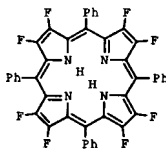
RN 131214-86-3 CAPLUS

CN 21H, 23H-Porphine, 2, 3, 7, 8, 12, 13, 17, 18-octabromo-5, 10, 15, 20-tetraphenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 87 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1997:790194 CAPLUS
 DOCUMENT NUMBER: 128:75218
 TITLE: 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetraphenylporphyrin: first synthesis and x-ray crystal structure of the ZnII complex
 AUTHOR(S): Leroy, Jacques; Bondon, Arnaud; Toupet, Loic; Rolando, Christian
 CORPORATE SOURCE: Ecole Normale Supérieure. Département de Chimie, URA CNRS 1679, Paris, F-75231, Fr.
 SOURCE: Chemistry--A European Journal (1997), 3(11), 1890-1893
 CODEN: CEUJED; ISSN: 0947-6539
 PUBLISHER: Wiley-VCH Verlag GmbH
 DOCUMENT TYPE: Journal
 LANGUAGE: English



AB 2,3,7,8,12,13,17,18-Octafluoro-5,10,15,20-tetraphenylporphyrin (I) was prepared from 3,4-difluoropyrrole and benzaldehyde under Lindsey conditions. An X-ray crystal structure study of its ZnII complex has shown that the macrocycle core is nonplanar, a result in apparent contradiction with a blue-shifted UV/Vis spectrum. The results reported here demonstrate that a wide range of β -octafluoro-meso-arylated porphyrins, a new class of highly electron-deficient ligands, are potentially accessible from 3,4-difluoropyrrole, thus opening the door to, inter alia, efficient and robust oxidation catalysts.

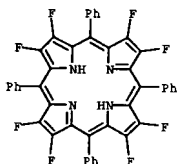
IT 186885-28-9P, 2, 3, 7, 8, 12, 13, 17, 18-Octafluoro-5, 10, 15, 20-tetraphenylporphyrin

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of octafluorotetraphenylporphyrin and the x-ray crystal structure of its zinc complex)

RN 186885-28-9 CAPLUS

CN 21H, 23H-Porphine, 2, 3, 7, 8, 12, 13, 17, 18-octafluoro-5, 10, 15, 20-tetraphenyl- (9CI) (CA INDEX NAME)

L6 ANSWER 87 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 88 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1997:723523 CAPLUS
 DOCUMENT NUMBER: 128:7724
 TITLE: Aggregation and axial ligand exchange behavior of water-soluble pyrrole- β brominated porphyrins
 AUTHOR(S): D'souza, Francis; Deviprasad, Gollapalli R.; Zandler, Melvin E.
 CORPORATE SOURCE: Department of Chemistry, The Wichita State University, Wichita, KS, 67260-0051, USA
 SOURCE: Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1997), (20), 3699-3703
 CODEN: JCOTBI; ISSN: 0300-9246
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Synthesis of two water-soluble pyrrole- β brominated porphyrins, the tetrachloro salt of 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(N-methyl-4-pyridinio)porphyrin [tetrakis(N-Me pyridyl)- β -octabromoporphyrin, (Br8TMPyP)H₂] and the tetrasodium salt of 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis-(Ph sulfonate)porphyrin [tetrakis(4-sulfonatophenyl)- β -octabromoporphyrin, (Br8TPPS)H₂] and their zinc(II) derivs. are reported. The investigated porphyrins are highly nonplanar due to the presence of eight bromo substituents at the pyrrole- β positions and four aryl groups at the meso positions. At I = 0.1M and T = 23°, the two sulfonated derivs., (Br8TPPS)H₂ and (Br8TMPyP)Zn show a small tendency to aggregate while such behavior is almost negligible for the N-Me pyridyl derivs. Like the unbrominated water-soluble zinc(II) porphyrin derivs., the pyrrole- β brominated zinc(II) porphyrins, with one or two water mols. as axial ligand(s) in aqueous

solution, undergo ligand exchange reactions with nitrogenous bases. The calculated equilibrium constant, K, for this reaction is smaller in magnitude when

compared to that obtained for the corresponding unbrominated zinc(II) porphyrin derivs. The equilibrium constant values parallel the basicity of the

axial ligands.

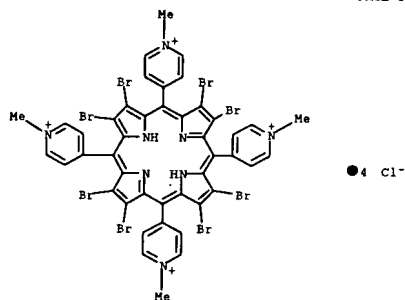
IT 198959-00-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and absence of aggregation behavior in aqueous solution)

RN 198959-00-1 CAPLUS

CN Pyridinium, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H, 23H-porphine-5,10,15,20-tetracyl)tetrakis[1-methyl-, tetrachloride, monohydrochloride (9CI) (CA INDEX NAME)

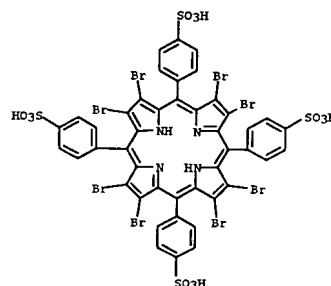
PAGE 1-A



PAGE 2-A

● HCl

PAGE 1-A



PAGE 2-A

REFERENCE COUNT:

58

THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

IT 198959-02-3P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and aggregation behavior in aqueous solution)

RN 198959-02-3 CAPLUS

CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis-, tetrasodium salt (9CI) (CA INDEX NAME)

L6 ANSWER 89 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:684406 CAPLUS

DOCUMENT NUMBER: 127:346236

TITLE: preparation of calixpyrroles, calixpyridinopyrroles and calixpyridines

INVENTOR(S): Gale, Philip A.; Sessler, Jonathan L.; Genge, John W.; Kral, Vladimir; Andriewsky, Andrei; Lynch, Vincent; Sansom, Petra I.; Allen, William E.; et al.

PATENT ASSIGNER(S): Board of Regents, the University of Texas System, USA

SOURCE: PCT Int. Appl., 145 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

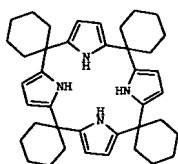
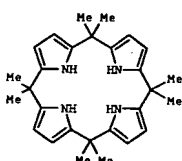
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9737995	A1	19971016	WO 1997-US5643	19970404
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2251072	AA	19971016	CA 1997-2251072	19970404
CA 2391030	AA	19971016	CA 1997-2391030	19970404
AU 9724409	A1	19971029	AU 1997-24409	19970404
EP 891364	A1	19990120	EP 1997-920143	19970404
R: CH, DE, FR, GB, IT, LI, NL, SE				
JP 2000511880	T2	20000912	JP 1997-536364	19970404
PRIORITY APPLN. INFO.:			US 1996-14890P	P 19960405
			US 1996-24203P	P 19960827
			US 1996-26694P	P 19960925
			US 1996-33395P	P 19961217
			US 1996-33396P	P 19961217
			CA 1997-2251072	A3 19970404
			WO 1997-US5643	W 19970404

OTHER SOURCE(S):

MARPAT 127:346236

GI



AB Preparation of calixpyrrole, calixpyridinopyrrole, and calixpyridine macrocycles having 4, 5, 6, 7, or 8 heterocyclic rings, such as I and II,

L6 ANSWER 89 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

was described. Such macrocycles have proved to be effective and selective ion- and neutral mol.-binding agents forming supramol. ensembles, and ion- and neutral mol.-sepn. agents. The macrocycles are fully meso-non-hydrogen-substituted porphyrinogens, a few mols. of which were previously known but not recognized as possessing anion- or mol.-binding properties. The binding mode is noncovalent, primarily that of hydrogen-bonding, thereby providing a new mode for liq. chromatog., that of hydrogen bonding liq. chromatog. Further useful applications of the macrocycles include environmental remediation by removal of undesired ions or neutral mols., and removal of phosphate for kidney dialysis. Thus, calix[4]pyrrole I was prepd. by cyclization of pyrrole and acetone in the presence of MeSO₃H, which was added slowly to prevent a violent reaction. II was prepd. by reaction of pyrrole with cyclohexanone in the presence of HCl. Stability consts. for I and II were detd. to demonstrate their affinity for various ions in soln., e.g. giving a const. of 350 ± 5.5 M⁻¹ for chloride.

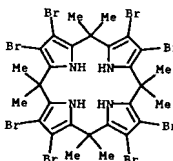
IT 190517-33-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); NUU (Other use, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of calixpyrroles, calixpyridinopyrroles and calixpyridines)

RN 190517-33-0 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1997:450915 CAPLUS
DOCUMENT NUMBER: 127:171539

TITLE: A potent superoxide dismutase mimic: manganese β -octabromo-meso-tetrakis-(N-methylpyridinium-4-yl) porphyrin
AUTHOR(S): Batinic-Haberle, Ines; Liochev, Stefan I.; Spasojevic, Ivana; Fridovich, Irwin
CORPORATE SOURCE: Department Biochemistry, Duke University Medical Center, Durham, NC, 27710, USA
SOURCE: Archives of Biochemistry and Biophysics (1997), 343(2), 225-233
CODEN: ABBIA4; ISSN: 0003-9861
PUBLISHER: Academic
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Various modified metalloporphyrins offer a promising route to stable and active mimics of superoxide dismutase (SOD). Here we explore bromination on the pyrroles as a means of increasing the redox potentials and the catalytic activities of the copper and manganese complexes of a cationic porphyrin. Mn(II) and Cu(II) octabrominated 5,10,15,20-tetrakis-(N-methylpyridinium-4-yl) porphyrin, MnIOBTMPyP4+, and CuIOBTMPyP4+ were prepared and characterized. The rate consts. for the porphyrin-catalyzed dismutation of O₂⁻ as determined from the inhibition of the cytochrome c reduction are k_{cat} = 2.2 + 108 and 2.9 + 106 M⁻¹ s⁻¹, i.e., IC₅₀ was calculated to be 12 nM and 0.88 μ M, resp. The metal-centered half-wave potential was E_{1/2} = +0.48 V vs NHE for the manganese compound CuIOBTMPyP4+ proved to be extremely stable, while its Mn(II) analog has a moderate stability, log K = 8.08. Nevertheless, slow manganese dissociation from MnIOBTMPyP4+ enabled the complex to persist and exhibit catalytic activity even at the nanomolar concentration level and at biol. pH. The corresponding MnIIIOBTMPyP5+ complex exhibited significantly increased stability, i.e., demetallation was not detected in the presence of a 400-fold molar excess of EDTA at micromolar porphyrin concentration and at

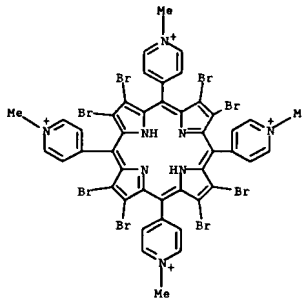
pH 7.8. The β -substituted manganese porphyrin facilitated the growth of a SOD-deficient strain of Escherichia coli when present at 0.05 μ M but was toxic at 1.0 μ M. The synthetic approach used in the case of manganese and copper compound offers numerous possibilities whereby the interplay of the type and of the number of β substituents on the porphyrin ring would hopefully lead to porphyrin compds. of increased stability, catalytic activity, and decreased toxicity.

IT 174580-26-8 174580-26-8D, protonated
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study) (superoxide dismutase mimic activity of manganese β -octabromo-meso-tetrakis-(N-methylpyridinium-4-yl) porphyrin)

RN 174580-26-8 CAPLUS
CN Pyridinium, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis[1-methyl-, tetrakis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

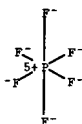
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CRN 174580-25-7
CMF C44 H30 Br8 N8



CM 2

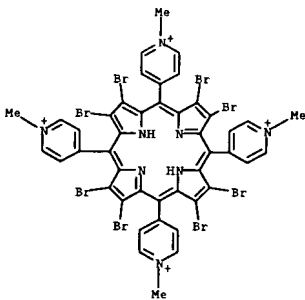
CRN 16919-18-9
CMF F6 P
CCI CCS



RN 174580-26-8 CAPLUS
CN Pyridinium, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis[1-methyl-, tetrakis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

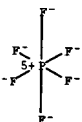
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CRN 174580-25-7
CMF C44 H30 Br8 N8



CM 2

CRN 16919-18-9
CMF F6 P
CCI CCS



ACCESSION NUMBER: 1997:330685 CAPLUS
DOCUMENT NUMBER: 126:350769

TITLE: First x-ray crystal structure of a lanthanide(III) monoporphyritic complex using non-planar porphyrin rings

AUTHOR(S): Spyroulias, Georgios A.; Despotopoulos, Alexis; Raptopoulou, Catherine P.; Terzis, Aris; Coutsolelos, Athanasios G.

CORPORATE SOURCE: Laboratory of Bioinorganic Coordination Chemistry, Department of Chemistry, School of Science, University of Crete, Heraklion, 714 09, Greece
SOURCE: Chemical Communications (Cambridge) (1997), (8), 783-784
CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

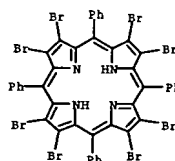
AB Twenty-three years after the 1st synthesis of lanthanide(III) porphyrins the x-ray crystal structure of [TbIII(β -C18tpp)(O2CMe)(Me2SO)2] is reported (H2tpp = 5,10,15,20-tetraphenylporphyrin; monoclinic, space group P21/c). The synthetic route to four halogenated porphyrins H2(β -Xntpp) (X = Cl or Br, n = 4 or 8) is described and compared with the corresponding [TbIII(β -Xntpp)(O2CMe)] complexes. The highly distorted structure of the TbIII complex is compared with similar perhalogenated porphyrinic complexes. The x-ray structure of the octabrominated free base is also reported.

IT 189874-66-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal structure)

RN 189874-66-6 CAPLUS
CN Formamide, N,N-dimethyl-, compd. with 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-21H,23H-porphine (2:1) (9CI) (CA INDEX NAME)

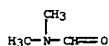
CM 1

CRN 131214-86-3
CMF C44 H22 Br8 N4

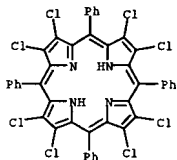


CM 2

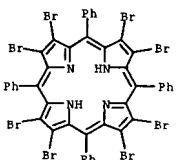
CRN 68-12-2
CMF C3 H7 N O



IT 120644-25-9P
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation, UV-visible spectrum and complexation with terbium)
 RN 120644-25-9 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



IT 131214-86-3P
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation, mol. structure, UV-visible spectrum and complexation with terbium)
 RN 131214-86-3 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

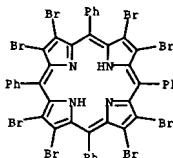


REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

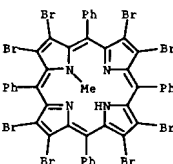
L6 ANSWER 92 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1997:318649 CAPLUS
 DOCUMENT NUMBER: 127:4955
 TITLE: Syntheses and structural properties of severely distorted porphyrins: N-methyl derivatives
 AUTHOR(S): Clement, Todd E.; Nguyen, Lien T.; Khoury, Richard G.; Nurco, Daniel J.; Smith, Kevin M.
 CORPORATE SOURCE: Dep. Chemistry, Univ. California, Davis, CA, 95616, USA
 SOURCE: Heterocycles (1997), 45(4), 651-658
 CODEN: HETCYM; ISSN: 0385-5414
 PUBLISHER: Japan Institute of Heterocyclic Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Syntheses and characterization of a series of N-methylated derivs. of sterically distorted porphyrins are reported; the work includes the first example of a tetra-N-methylated porphyrin obtained by methylation of an intact porphyrin.

IT 131214-86-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (syntheses and structural properties of severely distorted N-methylporphyrins)
 RN 131214-86-3 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

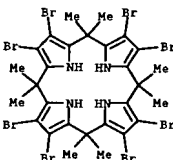


IT 190382-01-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (syntheses and structural properties of severely distorted N-methylporphyrins)
 RN 190382-01-5 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-21-methyl-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

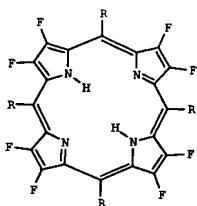
L6 ANSWER 93 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1997:275704 CAPLUS
 DOCUMENT NUMBER: 127:17652
 TITLE: Calix[4]pyrroles: C-rim substitution and tunability of anion binding strength
 AUTHOR(S): Gale, Philip A.; Sessler, Jonathan L.; Allen, William E.; Tvermoes, Nicolai A.; Lynch, Vincent
 CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of Texas at Austin, Austin, TX, 78712-1167, USA
 SOURCE: Chemical Communications (Cambridge) (1997), (7), 665-666
 CODEN: CHCOFS; ISSN: 1359-7345
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Electron-rich and electron-deficient C-rim substituted calix[4]pyrroles are synthesized and the anion binding ability of these receptors is found to be dependent upon the C-rim substituents.
 IT 190517-33-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and tunability of anion binding strength of calixpyrroles)
 RN 190517-33-0 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20,22,24-hexahydro-5,5,10,10,15,15,20,20-octamethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 1997:180900 CAPLUS
DOCUMENT NUMBER: 126:157325

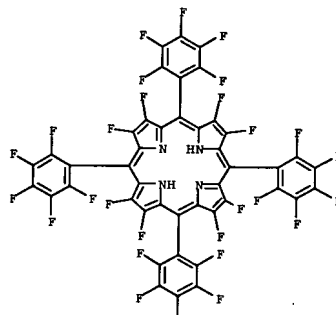
TITLE: 2,3,7,8,12,13,17,18-Octafluoro-5,10,15,20-tetraarylporphyrins and Their Zinc Complexes: First Spectroscopic, Electrochemical, and Structural Characterization of a Perfluorinated Tetraarylmetalloporphyrin
Woller, Eric K.; DiMaggio, Stephen G.
CORPORATE SOURCE: Department of Chemistry, University of Nebraska, Lincoln, NE, 68588-0304, USA
SOURCE: Journal of Organic Chemistry (1997), 62(6), 1588-1593
PUBLISHER: CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: American Chemical Society
LANGUAGE: English
GI



I

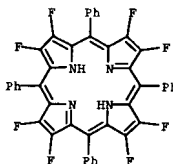
AB A convenient and general synthesis of β -octafluoroporphyrins I [R = Ph, C6F5, 3-MeOC6H4] is reported. The structural, spectroscopic, and electrochem. data indicate that β -octafluoro-meso-tetraarylporphyrins are a new class of planar, electron-deficient ligands. Particularly impressive is the 0.5 V window over which the formal oxidation potential can be tuned using only aryl substituents. The invariance of the ligand structure with increasingly pos. formal oxidation potential is a key advance;
electronic effects have been severed from the nonplanar conformations exhibited by all other highly electron-deficient porphyrins.
IT 121399-88-0P 186885-28-9P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and characterization of octafluorotetraarylporphyrins)
RN 121399-88-0 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

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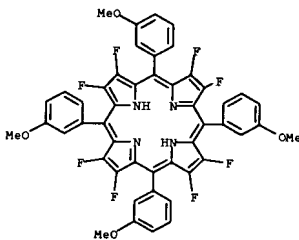


PAGE 2-A

RN 186885-28-9 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



IT 186885-29-0P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and characterization of octafluorotetraarylporphyrins)
RN 186885-29-0 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(3-methoxyphenyl)- (9CI) (CA INDEX NAME)

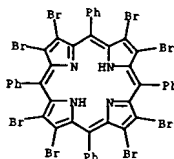


REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 1996:703905 CAPLUS
DOCUMENT NUMBER: 126:81682
TITLE: Nonlinear absorption in modified porphyrins
AUTHOR(S): Tang, N.; Su, W.; Cooper, T.; Adams, W.; Brandelik, D.; Brant, M.; McLean, D.; Sutherland, R.
CORPORATE SOURCE: Wright Lab, WL/MLPJ, WPAFB, OH, 45433, USA
SOURCE: Proceedings of SPIE-The International Society for Optical Engineering (1996), 2853(Nonlinear Optical Liquids), 149-157
CODEN: PSISDG; ISSN: 0277-786X
PUBLISHER: SPIE-The International Society for Optical Engineering
DOCUMENT TYPE: Journal
LANGUAGE: English

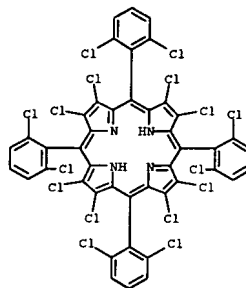
AB The authors study one free base and seven metallo-octabromotetraphenylporphyrins by several techniques. In a pico-second pump-probe experiment, the authors monitor the transient transmission of each sample up to 11 ns after it is irradiated by an intense laser pulse. Combined with the results from time-resolved fluorescence spectroscopy, the authors propose a simple model to interpret the transmission data. The authors attribute the reduction in the transmission to triplet state absorption and extract the triplet state absorption cross sections, as well as the lifetimes from the time dependent transmission data. In a sep. experiment where the transmission of a nanosecond laser pulse is measured with various input energies, the authors' measurement in the cross sections predicts the correct optical limiting behavior. The authors assess the overall optical limiting performance of all 8 samples by direct comparison with C60 at the same ground state transmission.

IT 131214-86-3
RL: PRP (Properties)
(nonlinear absorption and optical limiting for modified porphyrins)
RN 131214-86-3 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



L6 ANSWER 96 OF 148 CAPLUS COPYRIGHT 2005 ACS ON STN
 ACCESSION NUMBER: 1996:680693 CAPLUS
 DOCUMENT NUMBER: 126:67289
 TITLE: Photocatalytic oxidation of cyclohexane by (nBu4N)4W10032/Fe(III)porphyrins integrated systems
 AUTHOR(S): Maldotti, Andrea; Molinari, Alessandra; Bergamini, Paolo; Amadelli, Rossano; Battioni, Pierretter; Mansury, Daniel
 CORPORATE SOURCE: Dipartimento di Chimica, Centro di Studio su Fotoreattività e Catalisi del CNR, Università degli Studi di Ferrara, Via L. Borsari 46, Ferrara, 44100, Italy
 SOURCE: Journal of Molecular Catalysis A: Chemical (1996), 113(1-2), 147-157
 CODEN: JMCCF2; ISSN: 1381-1169
 PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The oxidation of cyclohexane by photoexcited (nBu4N)4W10032 has been investigated in the presence of iron meso-tetraarylporphyrins bearing different substituents in the β -pyrrole positions and/or in the meso-aryl groups. Irradiation at 325 nm leads to the reduction of the polyoxotungstate with the simultaneous oxidation of cyclohexane to cyclohexenyl radicals which can be detected by the ESR spin trapping technique. In oxygen-free solns., the photoreduced polyoxotungstate is able to transfer one electron to the Fe(III)porphyrin to give the ferrous complex. The subsequent reaction between this species and cyclohexenyl radicals leads to the formation of σ -alkyl-Fe(III)porphyrin complexes, as demonstrated by UV-visible and NMR spectroscopy. In the presence of oxygen, the photoreduced polyoxotungstate has the role of initiating the activation of O₂ through its reduction to O₂⁻ and H₂O₂. As a consequence, cyclohexane is converted to cyclohexanone and cyclohexanol in a cyclic way. The Fe(III)porphyrin complex strongly affects the product distribution probably through its hydrogen peroxide and alkyl-hydroperoxide-dependent oxidation. In comparison with (nBu4N)4W10032 alone, a higher selectivity is obtained with the formation of cyclohexanol as a major product.
 IT 134833-67-30, iron complexes
 RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process); PROC (Process); USES (Uses)
 (photocatalytic property of polyoxotungstate/iron tetraarylporphyrin system for oxidation of cyclohexane)
 RN 134833-67-3 CAPLUS
 CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(2,6-dichlorophenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 96 OF 148 CAPLUS COPYRIGHT 2005 ACS ON STN (Continued)



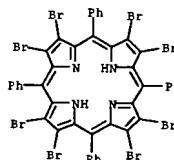
REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 97 OF 148 CAPLUS COPYRIGHT 2005 ACS ON STN
 ACCESSION NUMBER: 1996:674168 CAPLUS
 DOCUMENT NUMBER: 125:315678
 TITLE: Gas reactive pigment, gas detector using the same, and gas detection method and apparatus using the detector
 INVENTOR(S): Tanaka, Kazunari; Igarashi, Chiaki; Sadaoka, Yoshihiko
 PATENT ASSIGNEE(S): Ebara Corporation, Japan; Ebara Research Co., Ltd.
 SOURCE: Eur. Pat. Appl., 31 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 733901	A2	19960925	EP 1996-104433	19960320
EP 733901	A3	19961211		
R: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 09171011	A2	19970630	JP 1996-50431	19960307
TW 464651	B	20011121	TW 1996-85104567	19960417
PRIORITY APPLN. INFO.:				
JP 1995-85988 A 19950320				
JP 1995-270139 A 19951018				
JP 1996-50431 A 19960307				

OTHER SOURCE(S): MARPAT 125:315678
 AB A gas reactive pigment reactive to at least one of a halogen gas, a hydrogen halide gas, an acidic gas, an oxidizing gas, a basic gas, and an organic acid gas is provided. The pigment comprises a metal complex of tetraphenylporphyrin or a derivative thereof (I) wherein M represents a transition metal; a plurality of R's independently represent a hydrogen atom, a halogen atom, a nitro group, a cyano group or an alkoxy group, or a tetraphenylporphyrin derivative (II) wherein a plurality of R's independently represent a hydrogen atom, a halogen atom, a nitro group, a cyano group or an alkoxy group; a plurality of G's on the 4 Ph groups all represent a substituent selected from a halogen atom, a hydroxyl group, a sulfonic acid group, a carboxyl group, an alkoxy group, and an amino group, the positions of which on the 4 Ph groups may be the same or different; and a, b, c and d which may be the same or different, each represents an integer of 0 to 5, indicating the number of G's on each Ph group; provided that the compound wherein all R's represent a hydrogen atom, and a, b, c and d all represent 0 is excluded. A detector for the above gases containing the reactive pigment; a method for detecting the above gases using the detector; and a detection apparatus for the above gases using the detector are also provided. The gas reactive pigment shows a color change, which can be measured in terms of the absorption spectrum change of said pigment at high sensitivity on contact with the above gases.
 IT 131214-86-3, 2,3,7,8,12,13,17,18-Octabromo-5,10,15,20-tetraphenylporphyrin
 RL: ARG (Analytical reagent use); DEV (Device component use); ANST (Analytical study); USES (Uses)
 (gas anal. by detector based on tetraphenylporphyrin metal complexes)
 RN 131214-86-3 CAPLUS
 CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

L6 ANSWER 97 OF 148 CAPLUS COPYRIGHT 2005 ACS ON STN (Continued)

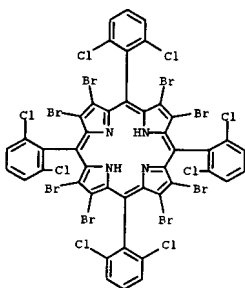


L6 ANSWER 98 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1996:673496 CAPLUS
 DOCUMENT NUMBER: 125:346125
 TITLE: Porphyrins bearing halogens at the meso-phenyl and
 β-pyrrolic positions: synthesis and spectral
 properties
 AUTHOR(S): Wijesekera, Tilak; Dupre, Daniel; Cader, Mohamed S.
 R.; Dolphin, David
 CORPORATE SOURCE: Dep. Chem., Univ. British Columbia, Vancouver, BC, V6T
 1Z1, Can.
 SOURCE: Bulletin de la Societe Chimique de France (1996),
 133(7-8), 765-775
 CODEN: BSCFAS; ISSN: 0037-8968
 PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The synthesis of sym. porphyrins chlorinated at both ortho positions of
 the meso-aryl substituents, and the chlorination and bromination of the
 β-pyrrolic positions is reported. The β-chlorination of
 meso-tetraphenylporphyrin via its nickel(II) complex is also described.
 The authors communicate the 1st perchlorination of tetramesitylporphyrin,
 where halogen substitution occurred at the β-pyrrolic positions as
 well as at both the vacant meta positions of the trimethylphenyl groups.
 The iron complexes of these various polyhalogenated porphyrins are also
 described, since they are robust and efficient catalysts in oxidation
 reactions.

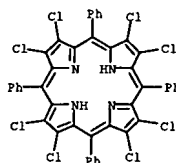
IT 107035-95-0P 120644-25-9P 131214-86-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and complexation with iron)

RN 107035-95-0 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,6-
 dichlorophenyl)- (9CI) (CA INDEX NAME)

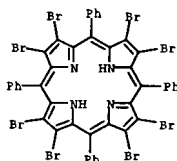


RN 120644-25-9 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-
 (9CI) (CA INDEX NAME)

L6 ANSWER 98 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

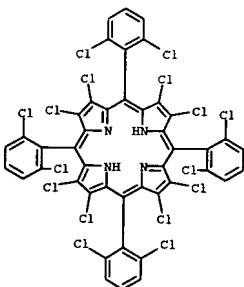


RN 131214-86-3 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-
 (9CI) (CA INDEX NAME)



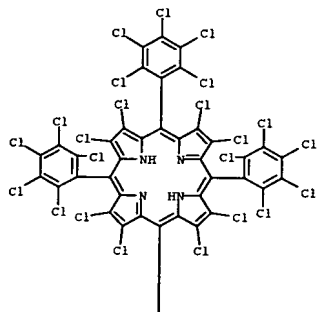
IT 134833-67-3P 183594-03-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 134833-67-3 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(2,6-
 dichlorophenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 98 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



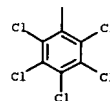
RN 183594-03-8 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-
 tetrakis(pentachlorophenyl)- (9CI) (CA INDEX NAME)

PAGE 1-A



L6 ANSWER 98 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 2-A

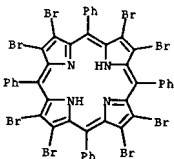


L6 ANSWER 99 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1996:552458 CAPLUS
 DOCUMENT NUMBER: 125:291504
 TITLE: meso-Substituted octabromoporphyrins: synthesis, spectroscopy, electrochemistry and electronic structure
 AUTHOR(S): Hariprasad, Gali; Dahal, Sanjay; Maiya, Bhaskar G.
 CORPORATE SOURCE: School Chemistry, University Hyderabad, Hyderabad, 500 046, India
 SOURCE: Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1996), (16), 3429-3436
 CODEN: JCDTBI; ISSN: 0300-9246
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The free-base, copper(II) and zinc(II) derivs. of 5,10,15,20-tetraarylporphyrin (aryl = Ph, 4-methylphenyl or 4-chlorophenyl) and the corresponding brominated 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraarylporphyrin derivs. were synthesized and their spectral and redox properties compared by UV/visible, ¹H NMR, ESR, and cyclic voltammetric methods. Substitution with the electron-withdrawing bromine groups at the pyrrole carbons has a profound influence on the UV/visible and ¹H NMR spectral features and also on the redox potentials of these systems. However, electron-withdrawing chloro or electron-donating Me groups at the para positions of the four Ph rings have only a marginal effect on the spectra and redox potentials of both the brominated and the nonbrominated derivs. The ESR data for the copper(II) derivs. of all these systems reveal that substitution at either the β -pyrrole carbons and/or the para positions of the meso-Ph groups does not significantly affect the spin-Hamiltonian parameters that describe the metal center in each case. Collectively, these observations suggest that the highest-occupied (HOMO) and lowest-unoccupied MOs (LUMO) of the octabromoporphyrins involve the porphyrin π -ring system as is the case with the nonbrominated derivs. Studies were carried out to probe the electronic structures of these systems by three different approaches involving spectral and redox potential data as well as AM1 calcs. The electron-withdrawing p-bromine substituents stabilize the LUMOs and, to a lesser degree, the HOMOs and the extent of these changes can be fine-tuned, in a subtle way, by substitution on the meso-aryl rings of a given porphyrin.

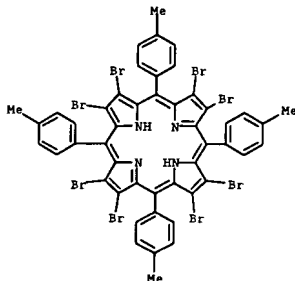
IT 131214-86-3
 RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent) (electronic structure and electrochem. redox of)

RN 131214-86-3 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

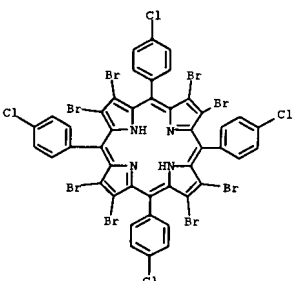


IT 182423-35-4P 182423-39-8P

L6 ANSWER 99 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn., complexation with copper or zinc, electronic structure and electrochem. redox of)
 RN 182423-35-4 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(4-methylphenyl)- (9CI) (CA INDEX NAME)



RN 182423-39-8 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(4-chlorophenyl)- (9CI) (CA INDEX NAME)



L6 ANSWER 100 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1996:422809 CAPLUS
 DOCUMENT NUMBER: 125:179700
 TITLE: Synthesis and electrochemistry of 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(3,5-dichloro-2,6-dimethoxyphenyl)porphyrin (H2tdcdmpp), [CoII(tdcdmpp)] and [M(tdcdmpp)Cl] (M = FeIII or MnIII)
 AUTHOR(S): Autret, Marie; Ou, Zhongping; Antonini, Alessandra; Boschi, Tristano; Tagliatesta, Peitro; Kadish, Karl M.
 CORPORATE SOURCE: Dep. Chem., Univ. Houston, Houston, TX, 77204-5641, USA
 SOURCE: Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1996), (13), 2793-2797
 CODEN: JCDTBI; ISSN: 0300-9246
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English

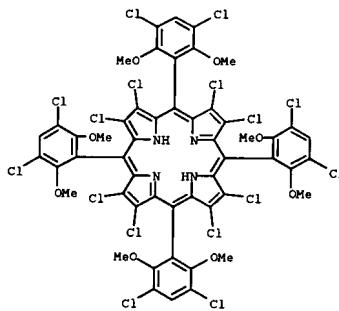
AB Four new highly chlorinated porphyrins, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(3,5-dichloro-2,6-dimethoxyphenyl)porphyrin (H2tdcdmpp), [CoII(tdcdmpp)] and [M(tdcdmpp)Cl] (M = FeIII or MnIII) were prepared. The free base was synthesized by chlorination of H2tdmpp (5,10,15,20-tetrakis(2,6-dimethoxyphenyl)porphyrin) and metalated to give the complexes following published procedures. The same transition-metal derivs. of tdmpp were also prepared and all eight synthesized compds. were electrochem. studied in benzonitrile or pyridine containing 0.1 mol dm⁻³ NBu₄ClO₄. As expected the half-wave potentials of the tdcdmpp complexes are shifted towards pos. values while those for oxidation or reduction of

the tdmpp species are shifted neg. as compared with E1/2 for oxidation or reduction of tetraphenylporphyrin (tpp) complexes having the same central metal ions. The magnitude of the anodic shifts in E1/2 for reduction with respect to tpp is among the largest reported for chlorinated porphyrins and ranges between 590 and 860 mV depending upon the specific redox reaction and solvent. A smaller $\Delta E1/2$ of 330-400 mV is seen for oxidation of the same compds. and these values can be compared to a negligible shift in E1/2 upon going from planar M(tpp) to distorted M(obtpp) (obtpp = 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenylporphyrinate) complexes of cobalt and iron where the effect of macrocycle ruffling is known to predominate over the electronic effects of added halide substituents. The core distortion cannot compensate totally for the electron-withdrawing effect of the Cl substituents. The macrocyclic distortion also induces a large red shift of the UV/visible absorption bands and this shift in λ_{max} ranges up to 40 nm for the chlorinated compds. with respect to the tdmpp complexes.

IT 180711-85-7P, 2,3,7,8,12,13,17,18-Octachloro-5,10,15,20-tetrakis(3,5-dichloro-2,6-dimethoxyphenyl)porphyrin
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and reaction with transition metal salts and elec. reduction potentials of)

RN 180711-85-7 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(3,5-dichloro-2,6-dimethoxyphenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 100 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



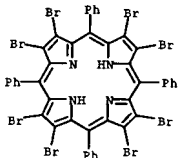
L6 ANSWER 101 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1996:396653 CAPLUS
 DOCUMENT NUMBER: 125:195272
 TITLE: Manifestation of structural features of porphyrin molecules in their electron absorption spectra
 AUTHOR(S): Berezin, D. B.; Andrianov, V. G.; Semelkin, A. S.
 CORPORATE SOURCE: Ivanovskaya Gosudarstvennaya Khimiko-Tekhnologicheskaya Akademiya, Ivanovo, 153460, Russia
 SOURCE: Optika i Spektroskopiya (1996), 80(4), 618-626
 CODEN: OPSPAM; ISSN: 0030-4034
 PUBLISHER: MAIK Nauka
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian

AB The suggested earlier hypothesis on the nature of the intense absorption band at 350-450 nm is discussed. This band may be caused by a photoinduced transfer of the electron d. from the pyrrole rings to the macrocyclic system. For porphyrins and their aza deriva. the information available from the value of the long-wave absorption band shift under protonation of the compds. is analyzed.

IT 131214-86-3P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and electronic structure of porphyrins by UV)

RN 131214-86-3 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



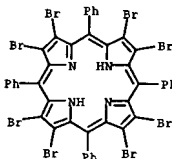
L6 ANSWER 102 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1996:306509 CAPLUS
 DOCUMENT NUMBER: 125:25070
 TITLE: Optochemical HCl and Cl2 gas detection based on tetraphenylporphyrine dispersed in ethyl-cellulose
 AUTHOR(S): Tagliatesta, Pietro; Sadaoka, Yoshihiko; Sakai, Yoshiro
 CORPORATE SOURCE: Dip. Sci. Technologie Chim., Univ. degli Roma, Tor Vergata, 00173, Italy
 SOURCE: Molecular Crystals and Liquid Crystals Science and Technology, Section A: Molecular Crystals and Liquid Crystals (1996), 278, 173-180
 CODEN: MCLCES; ISSN: 1058-725X
 PUBLISHER: Gordon & Breach
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB To detect sub-ppm levels of HCl gas, spectral changes of tetraphenylporphyrine and deriva. dispersed in ethylcellulose were examined in the visible region. For free base tetraphenylporphyrin, the absorbance at 450 nm and 670 nm is sensitive to sub-ppm levels of HCl and also a good reversibility is observed at room temperature. The Soret and Q-bands are insensitive to NH3, Cl2, NO2 and NO at room temperature. For zinc tetrabromotetraphenylporphyrine, the absorbance at 479 nm and 722 nm is sensitive to sub-ppm levels of HCl gas and also good reversibility is observed at room temperature.

IT 131214-86-3
 RL: PRP (Properties)
 (visible spectrum of)

RN 131214-86-3 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



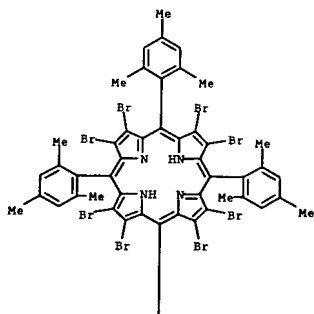
L6 ANSWER 103 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1996:290273 CAPLUS
 DOCUMENT NUMBER: 124:342946
 TITLE: Synthesis of β -Mono-, Tetra-, and Octasubstituted Sterically Bulky Porphyrins via Suzuki Cross Coupling
 AUTHOR(S): Zhou, Xiang; Tse, Man Kin; Wan, Terence S. M.; Chan, Kin Shing
 CORPORATE SOURCE: Departments of Chemistry, Chinese University of Hong Kong, Shatin, Hong Kong
 SOURCE: Journal of Organic Chemistry (1996), 61(11), 3590-3593
 CODEN: JOCEAH; ISSN: 0022-3263
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB β -Mono-, tetra-, and octa-substituted tetramesitylporphyrins were prepared in good yields by Suzuki cross-coupling reactions of β -bromotetramesitylporphyrins with aryl- and alkylboronic acids.

IT 129006-48-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (synthesis of sterically bulky porphyrins via Suzuki cross-coupling reactions)

RN 129006-48-0 CAPLUS

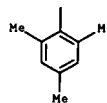
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)



PAGE 1-A

L6 ANSWER 103 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 2-A



L6 ANSWER 104 OF 148 CAPLUS COPYRIGHT 2005 ACS ON STN
 ACCESSION NUMBER: 1996:271551 CAPLUS
 DOCUMENT NUMBER: 124:316876
 TITLE: Haloporphyrins and their preparation
 INVENTOR(S): Ellis, Paul R., Jr.; Lyons, James E.
 PATENT ASSIGNEE(S): Sun Company, Inc. (R&D), USA
 SOURCE: Eur. Pat. Appl., 8 pp.
 CODEN: EFXNDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 11
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 700915	A1	19960313	EP 1995-306230	19950906
R: BE, DE, FR, GB, IT, NL				
CA 2157241	AA	19960308	CA 1995-2157241	19950830
JP 08113575	A2	19960507	JP 1995-254492	19950907
US 5663328	A	19970902	US 1996-672202	19960627
PRIORITY APPLN. INFO.:			US 1994-303106	A 19940907
			US 1987-246	A2 19870102
			US 1987-66666	A2 19870626
			US 1989-425089	B2 19891023
			US 1990-568116	A2 19900816

OTHER SOURCE(S): MARPAT 124:316876

AB The invention provides novel catalyst compns., useful in the oxidation of hydrocarbons with air or oxygen to form hydroxy-group containing compds. and in the decomposition of hydroperoxides to form hydroxy-group containing compds.

The catalysts comprise transition metal complexes of a porphyrin ring having 1 to 12 halogen substituents on the porphyrin ring, at least one of said halogens being in a meso position and/or the catalyst containing no aryl

group in a meso position. The compns. are prepared by halogenating a transition metal complex of a porphyrin. Thus, Cu porphyrin was chlorinated with Cl in CCl₄ to give the dodecachloroderiv. which was demetalated and then remetalated to give iron meso-tetrachloro- β -octachloroporphyrin chloride (I). I was used as a catalyst in the oxidation of isobutane to give mainly Me₃COH and in the decomposition of Me₃COOH to Me₃COH.

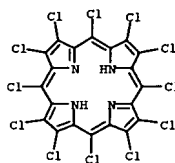
IT 144811-82-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of perhaloporphyrin complexes as oxidation catalysts)

RN 144811-82-5 CAPLUS

CN 21H,23H-Porphine, 2,3,5,7,8,10,12,13,15,17,18,20-dodecachloro- (9CI) (CA INDEX NAME)

L6 ANSWER 104 OF 148 CAPLUS COPYRIGHT 2005 ACS ON STN (Continued)



L6 ANSWER 105 OF 148 CAPLUS COPYRIGHT 2005 ACS ON STN
 ACCESSION NUMBER: 1996:247527 CAPLUS
 DOCUMENT NUMBER: 124:342944
 TITLE: En route to 2,3,7,8,12,13,17,18-octafluoroporphyrin
 AUTHOR(S): Leroy, Jacques
 CORPORATE SOURCE: Ec. Normale Supérieure, Dep. Chimie, Paris, 75231, Fr.
 SOURCE: Electronic Conference on Trends in Organic Chemistry [CD-ROM] (1996), Meeting Date 1995, Paper 40.
 Editor(s): Rzepa, Henry S.; Leach, Christopher; Goodman, Jonathan M. Royal Society of Chemistry: Cambridge, UK.
 CODEN: 62TKAB
 CONFERENCE
 DOCUMENT TYPE: English
 LANGUAGE:

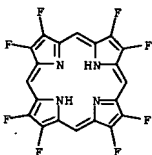
AB A symposium report with 13 refs. on the preparation of fluoropyrrole intermediates for octafluoroporphyrin.

IT 144811-86-9P

RL: PNU (Preparation, unclassified); PREP (Preparation)
 (preparation of intermediates for octafluoroporphyrin)

RN 144811-86-9 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro- (9CI) (CA INDEX NAME)



L6 ANSWER 106 OF 148 CAPLUS COPYRIGHT 2005 ACS ON STN
 ACCESSION NUMBER: 1996:182893 CAPLUS
 DOCUMENT NUMBER: 124:300066
 TITLE: Metalation of water-soluble octabromoporphyrin with lithium(I), cadmium(II), and mercury(II)
 AUTHOR(S): Tabata, Masaaki; Nishimoto, Jun; Ogata, Akiko; Kusano, Tohru; Nahar, Murun
 CORPORATE SOURCE: Dep. Chemistry, Saga Univ., Saga, 840, Japan.
 SOURCE: Bulletin of the Chemical Society of Japan (1996), 69(3), 673-77
 CODEN: BCSJAB; ISSN: 0009-2673
 PUBLISHER: Nippon Kagakai
 DOCUMENT TYPE: Journal
 LANGUAGE: English

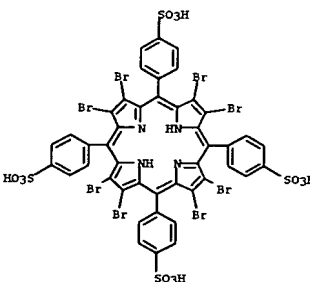
AB A water soluble porphyrin, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(4-sulfonatophenyl)porphyrin (H₂obtpps4-; H₂P4-) was synthesized and the equilibrium consts. were determined for the reaction of H₂obtpps4- with Li, Cd, and Hg(II) at 25° in I = 0.1 mol dm⁻³ (NaNO₃). The protonation consts. of H₂obtpps4- were determined. The porphyrin reacted with Li(I) in alkaline aqueous solution to form LiP5-, for which formation constant was determined. Na and K did not form their complexes under the same exptl. conditions. The equilibrium consts. for the formation of Cd(II) and Hg(II) porphyrins were determined. Hg(II) also forms homodinuclear porphyrin, Hg₂P4- for which the formation constant was determined. The octabromo groups lower the basicity of the porphyrin, which gave Li(I) porphyrin.

IT 154783-99-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (complexation with cadmium and mercury and lithium)

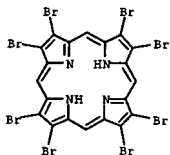
RN 154783-99-0 CAPLUS

CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis- (9CI) (CA INDEX NAME)

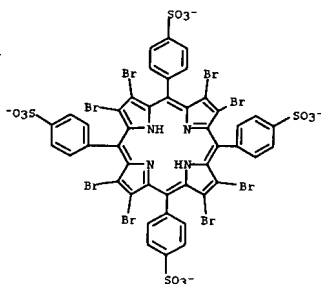


RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation,

L6 ANSWER 106 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
 nonpreparative)
 (formation consts.
 IT 144811-83-6P, 2,3,7,8,12,13,17,18-Octabromoporphyrin
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and sulfonation of)
 RN 144811-83-6 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo- (9CI) (CA INDEX NAME)



IT 176173-80-1
 RL: PRP (Properties)
 (protonation consts.)
 RN 176173-80-1 CAPLUS
 CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis-, ion(4-) (9CI) (CA INDEX NAME)



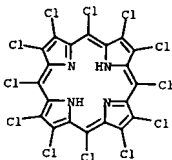
L6 ANSWER 107 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1996:161613 CAPLUS
 DOCUMENT NUMBER: 124:316505
 TITLE: Partial oxidation of hydrocarbons and decomposition of hydroperoxides catalyzed by haloporphyrin metal complexes
 INVENTOR(S): Ellis, Paul E., Jr.; Lyons, James E.
 PATENT ASSIGNER(S): Sun Co., Inc. (R and M), USA
 SOURCE: U.S., 5 pp. Cont.-in-part of U.S. Ser. No. 568,116.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 11
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5489716	A	19960206	US 1994-303105	19940907
US 4895682	A	19900123	US 1987-246	19870102
US 4900871	A	19900213	US 1987-66666	19870626
CA 1336188	A1	19950704	CA 1987-553420	19871203
US 5093491	A	19920303	US 1990-466163	19900117
CA 2157238	AA	19960308	CA 1995-2157238	19950830
EP 704447	A1	19960403	EP 1995-306231	19950906
JP 08104658	A2	19960423	JP 1995-254493	19950907
US 5663328	A	19970902	US 1996-672202	19960627

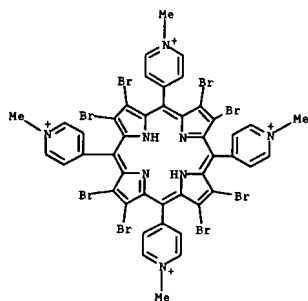
PRIORITY APPLN. INFO.:
 US 1987-246 A2 19870102
 US 1987-66666 A2 19870626
 US 1990-568116 A2 19900816
 US 1989-425089 B2 19891023
 US 1994-303105 A 19940907
 US 1994-303106 A3 19940907

OTHER SOURCE(S): CASREACT 124:316505; HARPAT 124:316505
 AB The invention provides novel methods for the oxidation of hydrocarbons with oxygen-containing gas to form hydroxy-group containing compds. and for the decomposition of hydroperoxides to form hydroxy-group containing compds.
 The catalysts used in the methods of the invention comprise transition metal complexes of a porphyrin ring having 1 to 12 halogen substituents on the porphyrin ring, at least one of said halogens being in a meso position and/or the catalyst containing no aryl group in a meso position. The catalyst compns. are prepared by halogenating a transition metal complex of a porphyrin. In one embodiment, a complex of a porphyrin with a metal whose porphyrin complexes are not active for oxidation of alkanes is halogenated, thereby to obtain a haloporphyrin complex of that metal, the metal is removed from the haloporphyrin complex to obtain the free base form of the haloporphyrin, and a metal such as iron whose porphyrin complexes are active for oxidation of alkanes and for the decomposition of alkyl hydroperoxides is complexed with the free base to obtain an active catalyst for oxidation of alkanes and decomposition of alkyl hydroperoxides. Thus, partial oxidation of isobutane with O2 catalyzed by iron complex of meso-tetrachloro-β-octachloroporphyrin (preparation given) afforded tert-Bu alc. as main product. Decomposition of tert-Bu hydroperoxide in tert-Bu alc. catalyzed by iron complex of meso-tetrachloro-β-octachloroporphyrin afforded tert-Bu alc.

L6 ANSWER 107 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
 IT 144811-82-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (partial oxidation of hydrocarbons and decomposition of hydroperoxides catalyzed by haloporphyrin metal complexes)
 RN 144811-82-5 CAPLUS
 CN 21H,23H-Porphine, 2,3,5,7,8,10,12,13,15,17,18,20-dodecachloro- (9CI) (CA INDEX NAME)



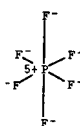
L6 ANSWER 108 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1996:145243 CAPLUS
 DOCUMENT NUMBER: 124:213140
 TITLE: Observation of a Stable Water-Soluble Lithium Porphyrin
 AUTHOR(S): Richards, Rosalie A.; Hammons, Kelly; Joe, Melanie; Miskelly, Gordon M.
 CORPORATE SOURCE: Department of Chemistry, University of Southern California, Los Angeles, CA, 90089-0744, USA
 SOURCE: Inorganic Chemistry (1996), 35(7), 1940-4
 CODEN: INOCAJ; ISSN: 0020-1669
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The deprotonated form of the water soluble porphyrin 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(N-methylpyridinium-4-yl)porphyrin, H2OBT(4-N-MePy)P4+, has a strong affinity for Li and forms a stable Li complex in basic aqueous solution. The fully deprotonated form, OBT(4-N-MePy)P2+, is present above pH 10 (pKa3 = 6.5 ± 0.1 and pKa4 = 10.2 ± 0.1). Li ions bind to this porphyrin in aqueous solution in a 1:1 stoichiometry with a binding constant of (9.6 ± 0.5) × 10² M⁻¹ (0.1M KOH, 298 K). The apparent binding constant for Li+ is reduced in the presence of a large excess of Na+, and a binding constant for Na+ of 1.0 ± 0.3M⁻¹ was obtained. The Li+ porphyrin in D2O shows a 7Li NMR signal at -10.25 ppm vs. 1.1M LiCl, and the line widths show exchange occurs at 299 K, in contrast to earlier Li porphyrins, which exchange more slowly. The Li-binding behavior and 7Li NMR spectra for 5,10,15,20-tetrakis(N-methylpyridinium-4-yl)porphyrin, HMT(4-N-MePy)P(2+x)+ (x = 0-2) are also reported.
 IT 174580-25-7P 174580-27-9P
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
 (preparation and binding consts. with lithium)
 RN 174580-25-7 CAPLUS
 CN Pyridinium, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis[1-methyl- (9CI) (CA INDEX NAME)



RN 174580-27-9 CAPLUS
 CN Pyridinium, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis[1-methyl-, tetrakis[hexafluorophosphate(1-)]], mono[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

CM 1

CRN 16940-81-1
 CMF F6 P . H
 CCI CCS



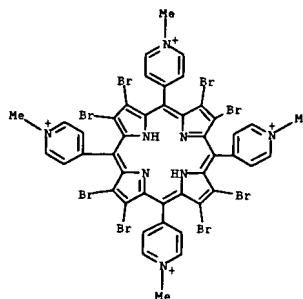
● H⁺

CM 2

CRN 174580-26-8
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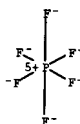
CM 3

CRN 174580-25-7



CM 4

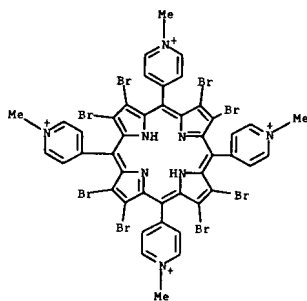
CRN 16919-18-9
 CMF F6 P
 CCI CCS



IT 174580-33-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 174580-33-7 CAPLUS
 CN Pyridinium, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis[1-methyl-, tetrachloride (9CI) (CA INDEX NAME)



● 4 Cl⁻

ACCESSION NUMBER: 1996:25316 CAPLUS
 DOCUMENT NUMBER: 124:101510
 TITLE: Energy Transfer and Electron Transfer of Poly(ethylene glycol)-Linked Fluorinated Porphyrin Derivatives in Lipid Bilayers
 AUTHOR(S): Nango, Mamoru; Iida, Kouji; Matsuura, Mitsutaka; Yamaguchi, Masashi; Sato, Kiyohito; Tanaka, Kazumasa; Akimoto, Kyoko; Yamashita, Keiji; Tsuda, Kazuichi; Kuroda, Yukihisa
 CORPORATE SOURCE: Department of Applied Chemistry, Nagoya Institute of Technology, Nagoya, 466, Japan
 SOURCE: Langmuir (1996), 12(2), 450-8
 CODEN: LANGD5; ISSN: 0743-7463
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Poly(ethylene glycol) [PEG]-linked porphyrin derivs. separated by spacer methylene groups (Cn), PEG-Cn-MFPFP (M = H2, Mn; n = 0, 5, 11), PEG-C11-MTTP (M = H2, Mn), and PEG-C0-MFPFP (M = H2, Mn) were synthesized. The porphyrin portion of the poly(ethylene glycol) [PEG]-linked fluorinated porphyrin derivative has been anchored onto a lipid bilayer. PEG-linked fluorinated porphyrins easily associated with phospholipid bilayers and are chemically stable against oxidants such as H2O2. An efficient energy transfer from phospholipid-linked zinc porphyrin, PE-C11-ZaFPPF to externally added PEG-Cn-H2FPPF (n = 0, 5, 11) in the lipid bilayer was observed, depending on the length of Cn and the porphyrin structure. Ground state transmembrane electron transfer especially when n = 11. Comparison of PEG-C11-MnFPPF- and PEG-C11-MnTTP-catalyzed electron transfer is made. The electron transfer rate was controlled not only by the separated spacer methylene groups between the porphyrin and PEG moieties but also by the structures of porphyrins.

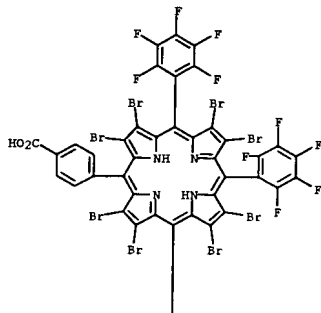
IT

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (in preparation of polyethylene glycol-linked fluorinated porphyrin derivs.)

RN 172663-37-5 CAPLUS

CN Benzoic acid, 4-(2,3,7,8,12,13,17,18-octabromo-10,15,20-tris(pentafluorophenyl)-21H,23H-porphin-5-yl)- (9CI) (CA INDEX NAME)

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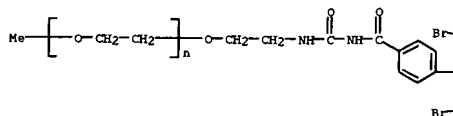


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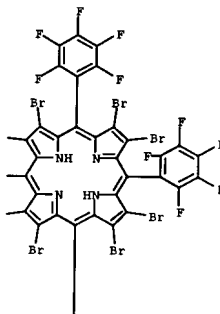


IT 172663-31-99
 RL: PEP (Physical, engineering or chemical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
 (photoinduced energy- and electron-transfer of polyethylene glycol-linked fluorinated porphyrin derivs. in lipid bilayers)
 RN 172663-31-9 CAPLUS
 CN Poly(oxy-1,2-ethanediyl), α -methyl- α -[2-[[[4-(2,3,7,8,12,13,17,18-octabromo-10,15,20-tris(pentafluorophenyl)-21H,23H-porphin-5-yl]benzoyl]amino]carbonyl]amino]ethoxy]- (9CI) (CA INDEX NAME)

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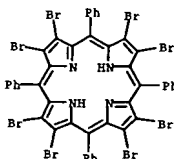
PAGE 1-B



PAGE 2-B



ACCESSION NUMBER: 1995:801155 CAPLUS
 DOCUMENT NUMBER: 123:305038
 TITLE: Synthesis and spectroscopic studies of lanthanide monophyrinates with meso-tetra-aryl porphyrinate bearing bromines on the β -pyrrole positions and fluorines on phenyl groups
 AUTHOR(S): Spyroulias, G. A.; Coutsolelos, A. G.
 CORPORATE SOURCE: Chemistry Dep., Univ. Crete, Crete, 71409, Greece
 SOURCE: Polyhedron (1995), 14(17/18), 2483-90
 CODEN: PLVHDE; ISSN: 0277-5387
 PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The metal derivs. of octabromotetraphenylporphyrin (H2obp) with lanthanide (Sm to Lu) ions were synthesized via the acetylacetonates and characterized by UV-visible, IR and ESR spectroscopies. These lanthanide complexes exhibit interesting electronic features compared with all the previously reported lanthanide monophyrinates. The stability of the complexes is discussed in terms of the already known related complexes. The meso-pentafluorophenyl-substituted porphyrin with SmIII was synthesized and its spectroscopic behavior compared with the above β -pyrrole octabromotetraphenyl complexes. IR studies indicate that the axial ligand is the acetylacetonate as was observed for lanthanide monophyrinates synthesized by the acetylacetonate method. ESR spectroscopy of Ln(obp)acac exhibit one intense peak with g approx. 2.00 and hyperfine splitting for Ln = Sm, Eu, Tb, Dy, Ho, Er, Tm, Yb, Lu. The ESR spectrum of Gd(obp)acac exhibits an isotropic g -factor with a value of 2.3099 and it compared with the analogous complex of Gd(tpp)acac.
 IT 131214-86-3P, 2,3,7,8,12,13,17,18-Octabromo-5,10,15,20-tetraphenylporphyrin
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (For preparation of rare earth meso-tetraphenyl-octabromoporphyrinato complexes)
 RN 131214-86-3 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



L6 ANSWER 111 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1995:718516 CAPLUS
 DOCUMENT NUMBER: 123:111720
 TITLE: Fast atom bombardment mass spectral observations on β -pyrrole-substituted tetraphenylporphyrins
 AUTHOR(S): Boschi, Tristano; D'Arcangelo, Giuseppe; Tagliatesta, Pietro
 CORPORATE SOURCE: Dep. di Scienze e Technologie Chimiche, Univ. degli Studi di Rome Tor Vergata, Rome, 00133, Italy
 SOURCE: Journal of Chemical Research, Synopses (1995), (8), 326-7
 CODEN: JRPSDC; ISSN: 0308-2342
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English

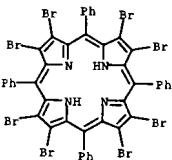
AB The FAB mass spectra of brominated porphyrins have been measured using different matrixes and the fragmentation patterns related to the acidity of the media.

IT 131214-86-3
 RL: FRP (Properties)

(Fast atom bombardment mass spectral observations on β -pyrrole-substituted tetraphenylporphyrins)

RN 131214-86-3 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



L6 ANSWER 112 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1995:716604 CAPLUS
 DOCUMENT NUMBER: 123:338859
 TITLE: Halogenated metalloporphyrin complexes as catalysts for selective reactions of acyclic alkanes with molecular oxygen
 AUTHOR(S): Lyons, James E.; Ellis, Paul E., Jr.; Myers, Harry K., Jr.
 CORPORATE SOURCE: Research and Developmental Department, Sun Company, Inc., Marcus Hook, PA, 19061-0835, USA
 SOURCE: Journal of Catalysis (1995), 155(1), 59-73
 CODEN: JCTLA5; ISSN: 0021-9517
 PUBLISHER: Academic
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 123:338859

AB We have shown that halogenation of the porphyrin ring of a metalloporphyrin complex can convert a catalytically inactive material into an exceptionally active catalyst for the selective reaction of an alkane with mol. oxygen. The greater the degree of halogenation of the ring, the greater is the catalytic activity of the metal complex. The product profile, while characteristic of radical reactions, is sensitive to the nature of the metal center. Iron complexes are generally more active than those of cobalt, manganese, or chromium. The activity of iron complexes is directly related to the Fe(III)/(II) reduction potential of the porphyrin complex. There is also a similar correlation between the Fe(III)/Fe(II) reduction potential and the rate at which iron haloporphyrin complexes decompose alkyl hydroperoxides. These iron perhaloporphyrin complexes are not only the most active known liquid phase alkane

air-oxidation catalysts, they are also the most active hydroperoxide decomposition catalysts known to date. The nature of the products formed is dependent on the structure of the aliphatic substrate that is oxidized and can be rationalized

by a catalytic pathway that very efficiently generates alkyl and alkoxy radicals at low temps. The relationship between the electrochem. properties of these complexes and the rates of alkane oxidation and hydroperoxide decomposition lends insight into possible mechanisms of catalytic activity.

IT 161405-60-3P

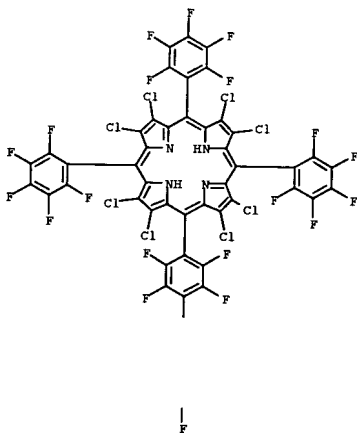
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (halogenated metalloporphyrin complexes as catalysts for alkane oxidation or alkyl hydroperoxide decomposition)

RN 161405-60-3 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 112 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

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L6 ANSWER 113 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1995:629765 CAPLUS
 DOCUMENT NUMBER: 123:186498
 TITLE: ¹⁹F NMR Spectra and Structures of Halogenated Porphyrins
 AUTHOR(S): Birnbaum, Eva R.; Hodge, Julia A.; Grinstaff, Mark W.; Schaefer, William P.; Henling, Lawrence; Labinger, Jay A.; Bercaw, John E.; Gray, Harry B.
 CORPORATE SOURCE: Arthur Amos Noyes Laboratory, California Institute of Technology, Pasadena, CA, 91125, USA
 SOURCE: Inorganic Chemistry (1995), 34(14), 3625-32
 CODEN: INOCAJ; ISSN: 0020-1669
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Fluorine-19 NMR spectra of a series of halogenated porphyrins have been used to create a spectral library of different types of fluorine splitting patterns for tetrakis(pentafluorophenyl) porphyrins (TFPP) complexed with diamagnetic and paramagnetic metal ions. The paramagnetic shift, line broadening, and fine structure of the resonances from the peripheral pentafluorophenyl rings are dependent on the symmetry and core environment of the porphyrin macrocycles. In combination with crystal structure data, ¹⁹F NMR helps define the behavior of halogenated porphyrins in solution. Six new crystal structures for TFPP and octahalo-TFPP derivs. are reported: H2TFPP in rhombohedral space group R.hivin.3, a = 20.327(4) Å, c = 24.368(5) Å, V = 8720(3) Å³, Z = 9; 2nTFPP in monoclinic space group P21/c, a = 12.653(4) Å, b = 11.883(5) Å, c = 15.261(2) Å, β = 103.87(2)°, V = 2227.6(13) Å³, Z = 9; CuTFPP in rhombohedral space group R.hivin.3, a = 20.358(5) Å, c = 24.347(6) Å, V = 8739(4) Å³, Z = 9; H2TFPPCl8 in triclinic space group P.hivin.1, a = 11.066(1) Å, b = 14.641(3) Å, c = 14.678(2) Å, α = 88.97(1)°, β = 76.05(1)°, γ = 71.29(1)°, V = 2181.4(6) Å³, Z = 2; 2nTFPPCl8 in tetragonal space group P.hivin.421c, a = 19.502(20) Å, c = 10.916(8) Å, V = 4152(6) Å³; H2TFPPBr8 in monoclinic space group C2, a = 27.634(6) Å, b = 6.926(2) Å, c = 14.844(3) Å, β = 109.64(2)°, V = 2675.8(11) Å³, Z = 2.

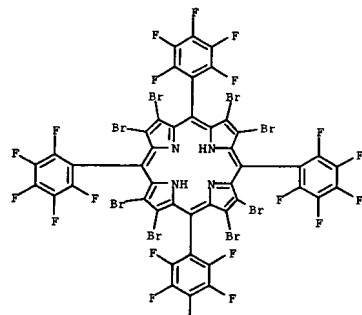
IT 139944-26-6P 161405-60-3P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (19F NMR spectra and structures of halogenated porphyrins)

RN 139944-26-6 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

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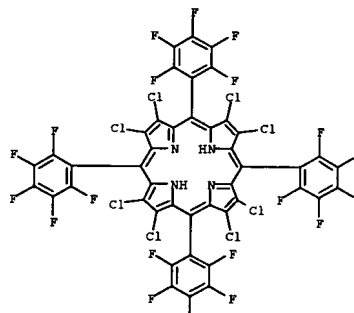


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RN 161405-60-3 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

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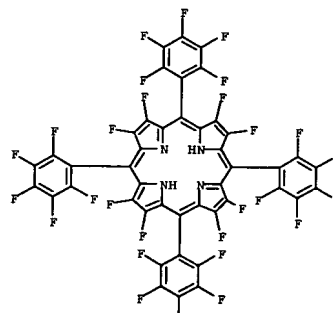


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L6 ANSWER 114 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
 RL: FRP (Properties)
 (local d. function study of substituent effects on valence ionization potentials of porphyrins)
 RN 121399-88-0 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

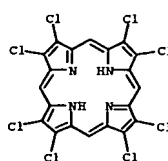
PAGE 1-A



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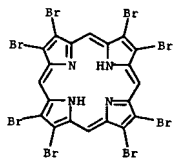
RN 144811-81-4 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro- (9CI) (CA INDEX NAME)



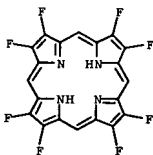
RN 144811-83-6 CAPLUS

L6 ANSWER 114 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1995:508382 CAPLUS
 DOCUMENT NUMBER: 122:290548
 TITLE: Substituent Effects on Valence Ionization Potentials of Free Base Porphyrins: A Local Density Functional Study
 AUTHOR(S): Ghosh, Abhik
 CORPORATE SOURCE: Department of Chemistry, University of Minnesota, Minneapolis, MN, 55455, USA
 SOURCE: Journal of the American Chemical Society (1995), 117(16), 4691-9
 CODEN: JACSAT; ISSN: 0002-7863
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Local d. functional (LDF) calcs. with polarized double- ζ basis sets have been used to calculate the two lowest one-electron ionization potentials
 (IPs) of a variety of free base porphyrins with multiple alkyl, aryl, fluoro, chloro, bromo, trifluoromethyl, cyano, and nitro substituents. For unsubstituted porphyrin (PH2), β -octaalkylporphyrins, and meso-tetraphenylporphyrin (TPPH2), LDF-ASCF calcs. reproduce the lowest UV photoelectron spectral (UPS) IPs to within \sim 0.2 eV. The two lowest one-electron IPs of TPPH2 are predicted to be lower than those of PH2 by \sim 0.5 eV, in agreement with UPS expts. Ab initio Hartree-Fock (HF) theory seriously underestimates this electronic effect of meso-tetra-Ph substitution. Both LDF and HF theories predict that substituents on the Ph rings of TPPH2 should strongly affect the lowest one-electron IPs of TPPH2. Substitution of the para positions of the Ph groups of TPPH2 with $-\text{CF}_3$, $-\text{CN}$, or $-\text{NO}_2$ substituents should raise the lowest IP by 0.7-0.8 eV, while perfluorination of the Ph rings should increase the lowest IP by \sim 0.95 eV. A comparison of the IPs of ortho-, meta-, and para-fluorinated TPPH2 derives suggests that electron-withdrawing substituents at meta and para positions should exert significantly stronger electronic effects on the porphyrin ring than ortho substituents. Ab initio HF theory seriously overestimates the electron-withdrawing effect of peripheral halogen substituents. Provided there is no macrocycle buckling due to steric interactions among peripheral substituents, LDF theory predicts that meso-tetrahalogenation (with F, Cl, or Br) should have almost no influence on the lowest IP of PH2, while β -octachlorination or octabromination should increase the lowest IP by \sim 0.4-0.5 eV. Electrochem. measurements support these LDF predictions. β -Octafluorination is predicted to exert an electronic effect of \sim 0.85 eV on the lowest IPs of PH2, which is significantly larger than the electronic effect of β -octachlorination or octabromination. Substituents such as $-\text{CF}_3$, $-\text{CN}$, and $-\text{NO}_2$ exert far higher electronic effects than the halogens. For instance, LDF theory predicts that the lowest IP of meso-tetrakis(trifluoromethyl)porphyrin should exceed that of TPPH2 by \sim 0.17 eV and that of meso-tetrakis(pentafluorophenyl)porphyrin by \sim 0.68 eV. Unlike the halogens, meso-tetra substitution with cyano groups should drastically increase the lowest IP of PH2, by a margin of \sim 0.12 eV. β -Octacyano-substitution is predicted to have an electronic effect of >2.0 eV on the lowest IP of PH2. Meso-tetranitrosubstitution is predicted to elevate the lowest IP of PH2 by \sim 0.9-1.1 eV, depending on the conformation of the nitro groups. In general, meso-substituents exert stronger electronic effects than the same substituents placed at β -positions.
 IT 121399-88-0 144811-81-4, Octachloroporphine
 144811-83-6, Octabromoporphine 144811-86-9, Octafluoroporphine

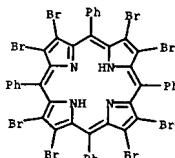
L6 ANSWER 114 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo- (9CI) (CA INDEX NAME)



RN 144811-86-9 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro- (9CI) (CA INDEX NAME)



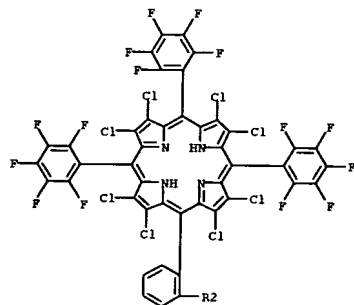
L6 ANSWER 115 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1995:476115 CAPLUS
 DOCUMENT NUMBER: 122:290549
 TITLE: Synthesis of beta-aryl substituted porphyrins by palladium catalyzed Suzuki cross-coupling reactions
 AUTHOR(S): Chan, Kin Shing; Zhou, Xiang; Au, Ming Tak; Tam, Chak Yue
 CORPORATE SOURCE: Department of Chemistry, The Chinese Univ. of Hong Kong, Shatin, Hong Kong
 SOURCE: Tetrahedron (1995), 51(11), 3129-36
 CODEN: TETRA; ISSN: 0040-4020
 PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 122:290549
 AB β -Bromoporphyrins undergo Suzuki cross coupling reactions with aryl boronic acids $p\text{-X-C}_6\text{H}_4\text{B(OH)}_2$ (X = H, Me, MeO, MeS, Cl) to give β -arylporphyrins in high yields.
 IT 131214-86-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of β -arylporphyrins by palladium-catalyzed Suzuki cross-coupling with arylboronic acids)
 RN 131214-86-3 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



L6 ANSWER 116 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1995:465601 CAPLUS
 DOCUMENT NUMBER: 122:223871
 TITLE: Metal complexes of substituted gable porphyrins as oxidation catalysts.
 INVENTOR(S): Lyons, James E.; Ellis, Paul E., Jr.; Wagner, Richard W.
 PATENT ASSIGNEE(S): Sun Co., Inc., USA
 SOURCE: Eur. Pat. Appl., 8 pp.
 CODEN: EFXKDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

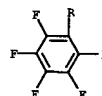
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 636628	A1	19950201	EP 1994-305634	19940729
R: BE, DE, FR, GB, IT, NL				
US 5480986	A	19960102	US 1993-100516	19930730
CA 2129055	AA	19950131	CA 1994-2129055	19940728
JP 07089964	A2	19950404	JP 1994-197953	19940729
			US 1993-100516	A 19930730

PRIORITY APPL. INFO.:
 OTHER SOURCE(S): MARPAT 122:223871
 AB Transition metal complexes of Gable porphyrins having two porphyrin rings connected through a linking group, and having on the porphyrin rings electron-withdrawing groups, such as halogen, nitro or cyano, are useful as catalysts for the oxidation of organic compds., e.g. alkanes.
 IT 162023-49-6P
 RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
 (metal complexes of substituted Gable porphyrins as oxidation catalysts)
 RN 162023-49-6 CAPLUS
 CN 21H,23H-Porphine, 5,5'-(1,2-phenylene)bis[2,3,7,8,12,13,17,18-octachloro-10,15,20-tris(pentafluorophenyl)- (9CI) (CA INDEX NAME)

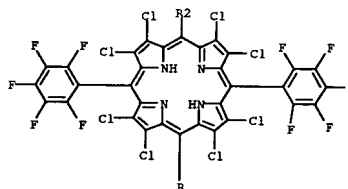


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L6 ANSWER 116 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



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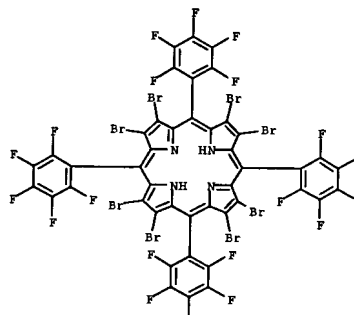


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L6 ANSWER 117 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1995:448372 CAPLUS
 DOCUMENT NUMBER: 122:203772
 TITLE: Electronic Structures of Halogenated Ruthenium Porphyrins. Crystal Structure of RuTFPPC18(CO)H2O (TFPPC18 = Octa- β -chlorotetrakis(pentafluorophenyl)porphyrin)
 AUTHOR(S): Birnbaum, Eva R.; Schaefer, William P.; Labinger, Jay A.; Bercaw, John E.; Gray, Harry B.
 CORPORATE SOURCE: Arthur Amos Noyes Laboratory, California Institute of Technology, Pasadena, CA, 91125, USA
 SOURCE: Inorganic Chemistry (1995), 34(7), 1751-5
 CODEN: INOCAL; ISSN: 0020-1669
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Ru(II) octa- β -halotetrakis(pentafluorophenyl)porphyrins (RuTFPPX8(CO), RuTFPPC18(py)2; X = Cl, Br) were synthesized, and the crystal structure of RuTFPPC18(CO)H2O was determined: monoclinic, space group P21/c, a 14.364(3), b 16.012(4), c 26.679(8) Å, β 90.29(2)°, Z = 4, R_w = 0.028 on F² for 8005 reflections, R = 0.067 for 5378 reflections with Fo₂ > 3 σ (Fo₂); the porphyrin is highly distorted, with a 1.19 Å maximum displacement of the β -Cl atoms from the mean porphyrin plane. The reduction potentials of RuTFPPX8 complexes are much more pos. (> 0.5 V) than those of unhalogenated analogs, owing to the influence of the electron-withdrawing X atoms. The relatively high energies of the Soret bands in the RuTFPPX8 electronic spectra are consistent with an electronic structural model involving RuII back-bonding to the porphyrin ex* orbitals.
 IT 139944-26-6, Octa- β -bromotetrakis(pentafluorophenyl)porphyrin
 161405-60-3, Octa- β -chlorotetrakis(pentafluorophenyl)porphyrin
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (for preparation of ruthenium halogenated porphyrinato complexes)
 RN 139944-26-6 CAPLUS
 CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 117 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

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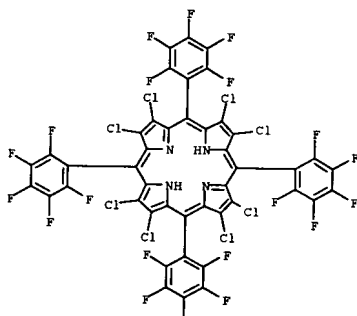


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RN 161405-60-3 CAPLUS
 CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 117 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

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L6 ANSWER 118 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1995:280591 CAPLUS
 DOCUMENT NUMBER: 122:187199
 TITLE: Sterically strained porphyrins - effect of nuclear protonation and peripheral substituents on the conformation in tetra-meso-, octa- β -, and dodeca-substituted porphyrin dications
 AUTHOR(S): Senge, Mathias O.; Forsyth, Timothy P.; Nguyen, Lien T.; Smith, Kevin M.
 CORPORATE SOURCE: Dep. Chem., Univ. California, Davis, CA, 95616, USA
 SOURCE: Angewandte Chemie (1994), 106(23/24), 2554-7 (See also Angew. Chem., Int. Ed. Engl., 1994, 33(23/24), 2485-7)
 CODEN: ANCEAD; ISSN: 0044-8249
 PUBLISHER: VCH
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 AB The conformations of meso-tetra-, β -octa-, and dodeca-substituted porphyrin dications are discussed.
 IT 161614-78-4
 RL: PRP (Properties)
 (effect of nuclear protonation and peripheral substituents on the conformation in tetra-meso-, octa- β -, and dodeca-substituted porphyrin dications)
 RN 161614-78-4 CAPLUS
 CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,13,20-tetraphenyl-, bis(trifluoroacetate), compd. with trichloromethane (2:1) (9CI) (CA INDEX NAME)
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 CRN 67-66-3
 CMF C H Cl3

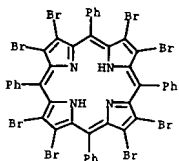


CM 2

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CM 3

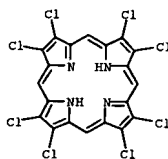
CRN 131214-86-3
 CMF C44 H22 Br8 N4



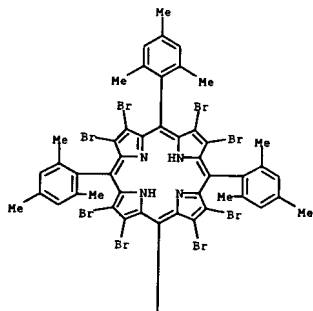
CM 4
CRN 76-05-1
CMF C2 H F3 O2



L6 ANSWER 119 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:114875 CAPLUS
DOCUMENT NUMBER: 122:160334
TITLE: Ab Initio Hartree-Fock and Local Density Functional Calculations on Prototype Halogenated Porphyrins. Do Electrochemically Measured Substituent Effects Reflect Gas-Phase Trends?
AUTHOR(S): Ghosh, Abhik
CORPORATE SOURCE: Department of Chemistry, University of Minnesota, Minneapolis, MN, 55455, USA
SOURCE: Journal of Physical Chemistry (1994), 98(43), 11004-6
CODEN: JPCHAX; ISSN: 0022-3654
DOCUMENT TYPE: Journal
LANGUAGE: English
AB First-principles quantum chemical methods have been employed to simulate and predict the electronic effects of peripheral polyhalogenation in porphyrins. Spin-RHF theory performs unexpectedly poorly in calcns. of valence ionization potential of polyhalogenated porphyrins. In contrast, the results of local d. functional calcns. of the lowest ionization potentials of free base porphyrin, meso-tetrafluoroporphyrin, and β -octachloroporphyrin are consistent with existing electrochem. information.
IT 144811-81-4, β -Octachloroporphyrin
RL: FRP (Properties)
(ab initio Hartree-Fock and local d. functional calcns. of substituent effects in halogenated porphyrins)
RN 144811-81-4 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro- (9CI) (CA INDEX NAME)

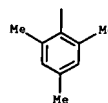


L6 ANSWER 120 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1994:700639 CAPLUS
DOCUMENT NUMBER: 121:300639
TITLE: Synthesis of β -octasubstituted sterically bulky porphyrins by Suzuki cross coupling
AUTHOR(S): Zhou, Xiang; Zhou, Zhong-yuan; Mak, Thomas C. W.; Chan, Kin Shing
CORPORATE SOURCE: Dep. Chem., Chin. Univ. Hong Kong, Shatin, Hong Kong
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1994), (18), 2519-20
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 121:300639
AB β -Octasubstituted tetramesitylporphyrins have been prepared in good yields by Suzuki cross coupling of β -octabromotetramesitylporphyrin with aryl- and alkyl-boronic acids. A single-crystal X-ray anal. of β -octamethyltetramesitylporphyrin shows a saddled non-planar structure.
IT 129006-48-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(Suzuki cross coupling with boronic acids)
RN 129006-48-0 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)



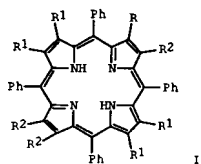
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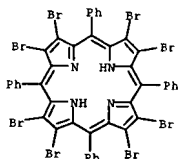


L6 ANSWER 121 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1994:435121 CAPLUS
 DOCUMENT NUMBER: 121:35121
 TITLE: Synthesis of β -aryl substituted porphyrins by palladium-catalyzed cross-coupling reactions
 AUTHOR(S): Chan, Kin Shing; Zhou, Xiang; Luo, Bao Sheng; Mak, Thomas C. W.
 CORPORATE SOURCE: Dep. Chem., Chin. Univ. Hong Kong, Shatin, Hong Kong
 SOURCE: Journal of the Chemical Society, Chemical Communications (1994), (3), 271-2
 CODEN: JCCCAT; ISSN: 0022-4936
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

L6 ANSWER 121 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



AB β -Bromoporphyrins I (R = Br, R1 = R2 = H; R = R2 = H, R1 = Br; R = R1 = R2 = Br) undergo Suzuki cross-coupling reactions with aryl boronic acids to give β -arylporphyrins I (R = Ar, R1 = R2 = H; R = R2 = H, R1 = Ar; R = R1 = R2 = Ar; Ar = Ph, 4-MeC6H4, 4-MeOC6H4, 4-Me3CC6H4, 4-ClC6H4) in high yields and x-ray anal. shows that H2TPP(Ph)4 I (R = R2 = H, R1 = Ph) (TPP = tetraphenylporphyrin) is centrosym. and possesses a hydrogen-bonded inner core.
 IT 131214-86-3
 RL: PRP (Properties)
 (palladium-catalyzed cross-coupling of, with aryl boronic acids)
 RN 131214-86-3 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

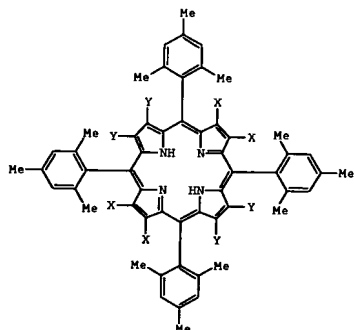


L6 ANSWER 122 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1994:435117 CAPLUS
 DOCUMENT NUMBER: 121:35117
 TITLE: Effect of conformation on the redox potentials of porphyrins halogenated in the β -pyrrole positions
 AUTHOR(S): Ochsenbein, Philippe; Ayougou, Khadija; Mandon, Dominique; Fischer, Jean; Weiss, Raymond; Austin, Rachel N.; Jayaraj, Karupiah; Gold, Avram; Turner, James; Fajer, Jack
 CORPORATE SOURCE: Inst. Le Bel, Univ. Louis Pasteur, Strasbourg, F-67070, Fr.
 SOURCE: Angewandte Chemie (1994), 106(3), 355-7 (See also Angew. Chem., Int. Ed. Engl., 1994, 106(3), 348-50)
 CODEN: ANCEAD; ISSN: 0044-8249
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 GI

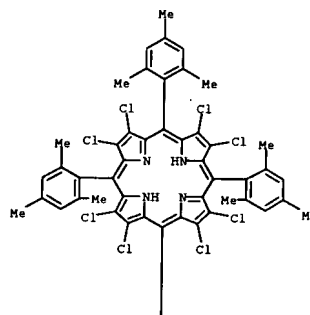
L6 ANSWER 122 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

CH 1
 CRN 152037-87-1
 CMF C56 H46 Cl8 N4

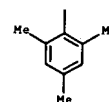
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AB The porphyrins I [X = Y = H, Cl, Br; X = Cl, Br, Y = H] were prepared and their redox potentials and crystal structures were compared. Increasing halogenation in I is accompanied by increasing twist in the mol. I [X = Cl, Br, Y = H, X] were more difficult to reduce than I [X = Y = H], but I [X = Y = Cl, Br] were more easily oxidized than I [X = Cl, Br, Y = H].
 IT 155586-24-6P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and crystal structure of)
 RN 155586-24-6 CAPLUS
 CN Methanol, compd. with 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)-21H,23H-porphine (2:1) (9CI) (CA INDEX NAME)



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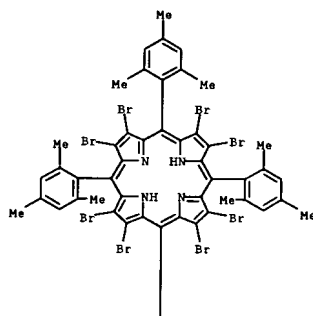


CH 2
 CRN 67-56-1
 CMF C H4 O

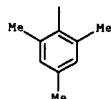
H3C-OH

IT 129006-48-0P 152037-87-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation, redox potential, and conformation of)
 RN 129006-48-0 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,4,6-

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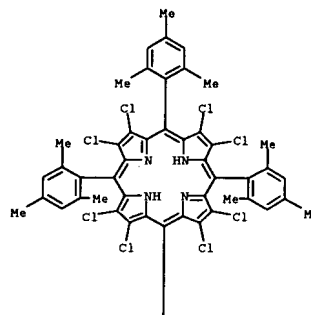


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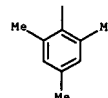


RN 152037-87-1 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

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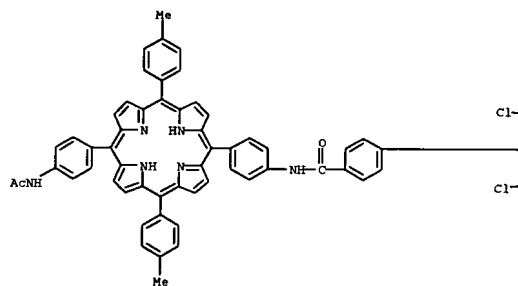


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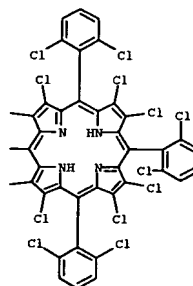


L6 ANSWER 123 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1994:311114 CAPLUS
DOCUMENT NUMBER: 120:311114
TITLE: Free Energy Dependence of Photoinduced Charge Separation Rates in Porphyrin Dyads
AUTHOR(S): DeGraziano, Janice M.; Liddell, Paul A.; Leggett, Lana; Moore, Ana L.; Moore, Thomas A.; Gust, Devens
CORPORATE SOURCE: Center for the Study of Early Events in Photosynthesis, Arizona State University, Tempe, AZ, 85287, USA
SOURCE: Journal of Physical Chemistry (1994), 98(7), 1758-61
DOCUMENT TYPE: CODEN: JPCHAX; ISSN: 0022-3654
LANGUAGE: English
AB A series of covalently linked porphyrin dyads in which the thermodyn. driving force for interporphyrin photoinduced charge separation spans a range of 1.13 eV has been prepared. Time-resolved fluorescence studies have yielded 22 rate consts. for photoinduced electron transfer in dichloromethane solution ranging from 4.1×10^7 to 5.0×10^{11} s⁻¹. The data are consistent with the theor. treatments of R. Marcus (1956) and V. Levich (1966), although there is no evidence for inverted behavior. In the normal region, electron transfer between free base porphyrin moieties is about 4 times faster than transfer involving a zinc porphyrin and having the same thermodyn. driving force, based on electrochem. measurements. Photoinduced electron transfer to an excited singlet state and electron transfer from an excited singlet state have the same dependence upon free energy change.
IT 154891-85-7 154891-86-8 154891-87-9
154896-34-2 154896-35-3 155208-76-7
RL: PRP (Properties)
(photoinduced intramol. electron transfer in, free energy dependence of)
RN 154891-85-7 CAPLUS
CN Benzamide, N-[4-[15-[4-(acetylamino)phenyl]-10,20-bis(4-methylphenyl)-21H,23H-porphin-5-yl]phenyl]-4-[2,3,7,8,12,13,17,18-octachloro-10,15,20-tris(2,6-dichlorophenyl)-21H,23H-porphin-5-yl]- (9CI) (CA INDEX NAME)

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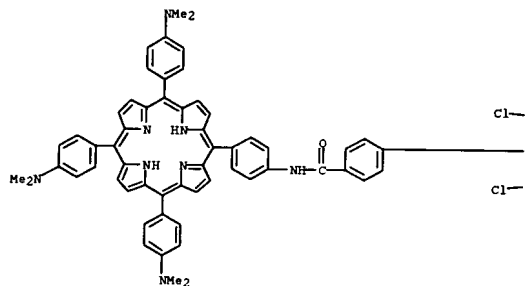


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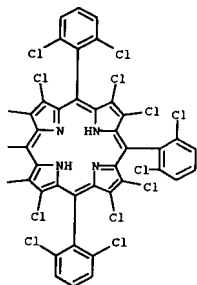


RN 154891-86-8 CAPLUS
CN Benzamide, 4-[2,3,7,8,12,13,17,18-octachloro-10,15,20-tris(2,6-dichlorophenyl)-21H,23H-porphin-5-yl]-N-[4-[10,15,20-tris(4-(dimethylamino)phenyl)-21H,23H-porphin-5-yl]phenyl]- (9CI) (CA INDEX NAME)

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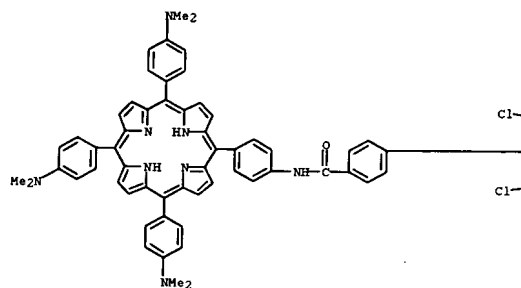


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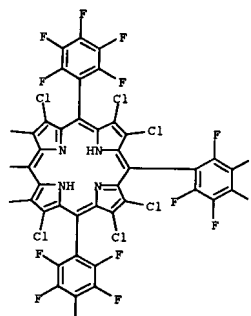


RN 154891-87-9 CAPLUS
 CN Benzamide, 4-[2,3,7,8,12,13,17,18-octachloro-10,15,20-tris(pentafluorophenyl)-21H,23H-porphin-5-yl]-N-[4-[10,15,20-tris(4-(dimethylamino)phenyl)-21H,23H-porphin-5-yl]phenyl]- (9CI) (CA INDEX NAME)

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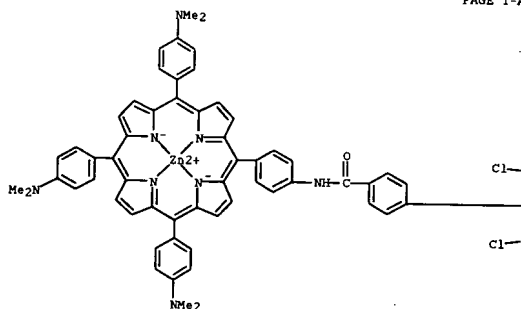
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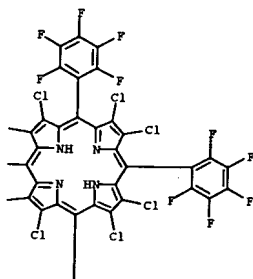
RN 154986-34-2 CAPLUS

CN Zinc, [4-[2,3,7,8,12,13,17,18-octachloro-10,15,20-tris(pentafluorophenyl)-21H,23H-porphin-5-yl]-N-[4-[10,15,20-tris(4-(dimethylamino)phenyl)-21H,23H-porphin-5-yl]phenyl]benzamidato(2-)-], (SP-4-2)- (9CI) (CA INDEX NAME)

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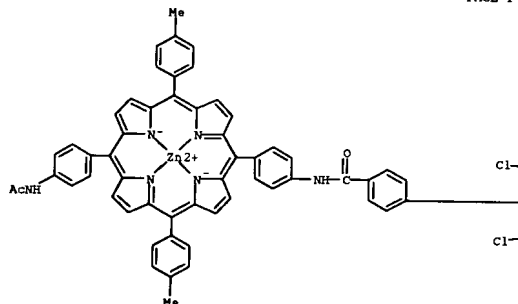
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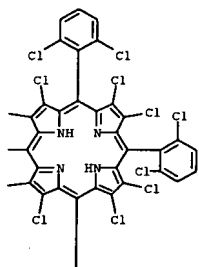
RN 154986-35-3 CAPLUS

CN Zinc, [N-[4-[15-[4-(acetylamino)phenyl]-10,20-bis(4-methylphenyl)-21H,23H-porphin-5-yl]phenyl]-4-[2,3,7,8,12,13,17,18-octachloro-10,15,20-tris(2,6-dichlorophenyl)-21H,23H-porphin-5-yl]benzamidato(2-)-], (SP-4-2)- (9CI) (CA INDEX NAME)

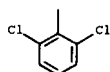
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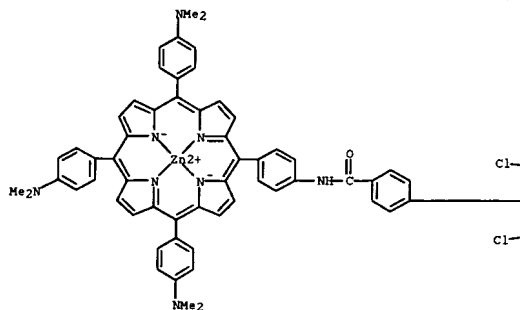


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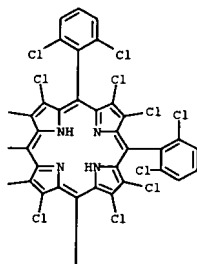


RN 155208-76-7 CAPLUS
 CN Zinc, [4-[2,3,7,8,12,13,17,18-octachloro-10,15,20-tris(2,6-dichlorophenyl)-21H,23H-porphin-5-yl]-N-[4-[10,15,20-tris(4-(dimethylamino)phenyl)-21H,23H-porphin-5-yl]phenyl]benzamidato(2-)]-, (SP-4-2)- (9Cl) (CA INDEX NAME)

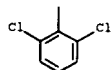
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L6 ANSWER 124 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1994:283247 CAPLUS
 DOCUMENT NUMBER: 120:283247
 TITLE: Resonance light-scattering studies of porphyrin diacid aggregates
 AUTHOR(S): Pasternack, Robert F.; Schaefer, Kurt F.; Hambright, Peter
 CORPORATE SOURCE: Department of Chemistry, Swarthmore College, Swarthmore, PA, 19081, USA
 SOURCE: Inorganic Chemistry (1994), 33(9), 2062-5
 CODEN: INOCAJ; ISSN: 0020-1669
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Resonance light scattering measurements were used to investigate the solute species present in acidic aqueous media for some 14 sulfonated porphyrins. The anomalous absorption band in the Soret region reported for several of these porphyrins arises from the formation of extended aggregates of electronically coupled chromophores and illustrate the sensitivity and specificity of this unconventional light scattering method.

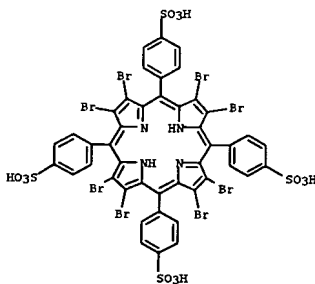
IT 154783-99-0

RL: PRP (Properties)

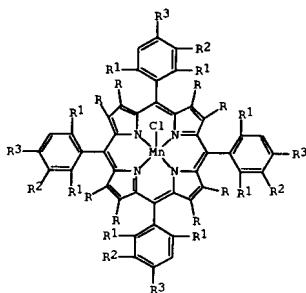
(resonance light scattering visible spectra of aggregates of)

RN 154783-99-0 CAPLUS

CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octabromo-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis- (9Cl) (CA INDEX NAME)



L6 ANSWER 125 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1994:134113 CAPLUS
 DOCUMENT NUMBER: 120:134113
 TITLE: Catalytic activity and chemical stability of perhalogenated manganese(II)-tetraarylporphyrins in alkene epoxidations
 AUTHOR(S): Banfi, Stefano; Mandelli, Roberto; Montanari, Fernando; Quici, Silvio
 CORPORATE SOURCE: Dip. Chim. Org. Ind., Univ. Milano, Milano, I-20133, Italy
 SOURCE: Gazzetta Chimica Italiana (1993), 123(7), 409-15
 CODEN: GCITA9; ISSN: 0016-5603
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

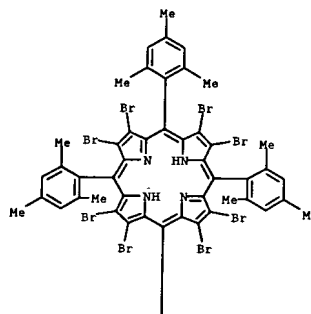


I

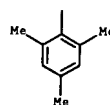
AB Structural factors, which govern the chemical stability of metallotetraarylporphyrins I (R = H, Cl, R1 = Cl, R2 = H, NO2, R3 = H; R = H, Br, R1 = R3 = Me, R2 = H; R = Me, R1 = Cl, R2 = R3 = H) were investigated in CH2Cl2/H2O two-phase alkene epoxidns. promoted by aqueous NaOCl or 30% H2O2. In contrast to recent literature reports, the perhalogenation of pyrrole β -positions of tetraarylporphyrins decreases the reactivity and the robustness of these catalysts with respect to the unsubstituted ones. The only exception is provided by I (R = Br, R1 = R3 = Me, R2 = H, II), which proved to be more efficient than I (R = H, R1 = R3 = Me, R2 = H). Nevertheless II is far less reactive than I (R = R2 = R3 = H, R1 = Cl). The influence of external factors, such as Mn-porphyrin/oxidant/substrate ratios and that of the axial ligand, was also examined. It was demonstrated that the assessed stability of polyhalogenated tetraarylporphyrins is subject to operative conditions where a large excess of substrate is used with respect to the oxidant, conditions which are difficult to use on a preparative scale.
 IT 129006-48-OP 134833-67-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)

L6 ANSWER 125 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
 (intermediate in prepn. of perhalogenated manganese(II)-tetraarylporphyrins)
 RN 129006-48-0 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

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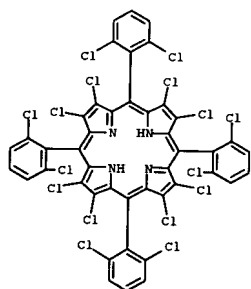


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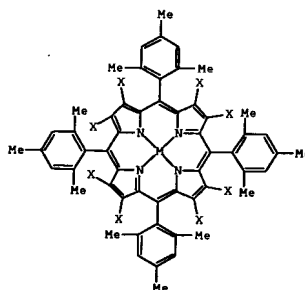


RN 134833-67-3 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(2,6-dichlorophenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 125 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



L6 ANSWER 126 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1994:67865 CAPLUS
 DOCUMENT NUMBER: 120:67865
 TITLE: The oxoiron π cation radical of meso-tetramesitylporphyrin chlorinated in the eight β positions: electronic and structural properties
 AUTHOR(S): Ochsenbein, Philippe; Mandon, Dominique; Fischer, Jean; Weiss, Raymond; Austin, Rachel; Jayaraj, Karupiah; Gold, Avram; Turner, James; Bill, Eckhardt; et al.
 CORPORATE SOURCE: Inst. LeBel, Univ. Louis Pasteur, Strasbourg, F-67070, Fr.
 SOURCE: Angewandte Chemie (1993), 105(10), 1504-5 (See also Angew. Chem., Int. Ed. Engl., 1193, 32(10), 1437-39)
 CODEN: ANCEAD; ISSN: 0044-8249
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 GI

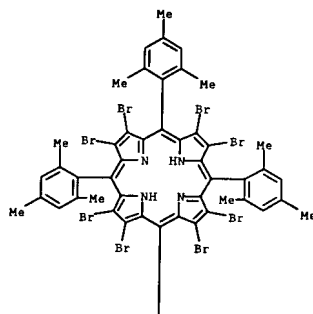


I

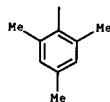
AB I (M = FeCl, X = Cl, Br) were prepared by the metalation of I (M = H2) with FeCl2. I.H2O are tetragonal, space group P41212, Z = 2, R/Rw = 0.069/0.091 and 0.053/0.075, resp. The Fe in I (M = FeCl, X = Cl, Br) lies 0.55(1) Å above the plane of the 4 N atoms. The average deviations of the β -C atoms from the plane are 0.87 and 0.90 Å for I (M = FeCl, X = Cl, Br), resp., in comparison to 0.90 and 0.95 Å for I (M = H2, X = Cl, Br), resp. I (M = FeCl, X = Cl, Br) were oxidized by m-chloroperoxybenzoic acid at -80° to give in toluene I (M = FeO, X = Cl, Br) which were ESR-inactive but in CH2Cl2 ESR-active I+ (M = FeO, X = Cl) was observed. The ESR data for I+ (M = FeO, X = Cl) is typical for a quartet ground state of S1 = 3/2 and indicated that ferromagnetic coupling occurs between the low-spin Fe(IV) center and the porphyrin π -radical cation. The temperature dependence of the exchange coupling is described using the 3-state model of the Kramer-doublet. Comparison of the spectral properties of I+ (M = FeO, X = Cl) with those of I+ (M = FeO, X = H) indicate that they have similar

L6 ANSWER 126 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
 electronic structures.
 IT 129006-48-0P 152037-87-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and mol. structure and oxidation of, by peroxybenzoic acid)
 RN 129006-48-0 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

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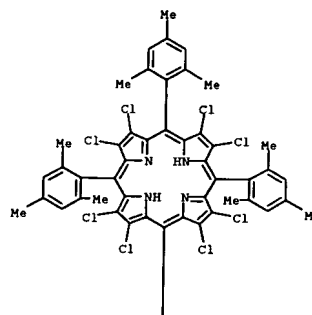


PAGE 2-A

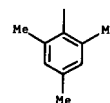


L6 ANSWER 126 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

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RN 152037-87-1 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

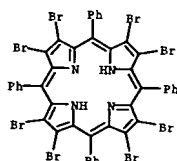
L6 ANSWER 127 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1993:594357 CAPLUS
 DOCUMENT NUMBER: 119:194357
 TITLE: Electrochemical and spectroelectrochemical behavior of cobalt(III), cobalt(II), and cobalt(I) complexes of meso-tetraphenylporphyrinate bearing bromides on the β -pyrrole positions
 AUTHOR(S): D'Souza, Francis; Villard, Anne; Van Caemelbecke, Eric; Franzen, Michelle; Boschi, Tristano; Tagliatesta, Pietro; Kadish, Karl M.
 CORPORATE SOURCE: Dep. Chem., Univ. Houston, Houston, TX, 77204-5641, USA
 SOURCE: Inorganic Chemistry (1993), 32(19), 4042-8
 CODEN: INOCAJ; ISSN: 0020-1669
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The synthesis and characterization of (meso-tetraphenylporphyrinato)cobalt(II) complexes containing 6, 7, or 8 Br groups at the β -pyrrole positions of the macrocycle are reported. Each compound undergoes 3 1-electron oxidns. and up to 9 1-electron redns. depending upon the degree of Br substitution. The 1st oxidation yields $[(\text{TPP})\text{Br}_x\text{Co(II)}]^+$ while the 1st reduction gives $[(\text{TPP})\text{Br}_x\text{Co(I)}]^-$ where (TPP)Br_x is the dianion of the brominated tetraphenylporphyrin. Cyclic voltammetry studies reveal a pos. shift of the metal and ring-centered redox potentials of the bromo porphyrins as compared to E_{1/2} for the reduction and oxidation of unsubstituted

(TPP)Co. The optical absorption spectra of each electrogenerated Co(I) and Co(III) complex were recorded in a thin-layer cell and show that the transition energies for both the Soret and visible bands vary as a function of Br groups on the porphyrin periphery. The electron withdrawing Br substituents also produce a red shift in the Soret and visible bands of the porphyrin which follows the order: $[(\text{TPP})\text{Br}_8\text{Co}] > [(\text{TPP})\text{Br}_7\text{Co}] > [(\text{TPP})\text{Br}_6\text{Co}] > [(\text{TPP})\text{Co}]$. The singly oxidized and singly reduced products are stable on the cyclic voltammetric and thin-layer times scales, but further reduction beyond $[(\text{TPP})\text{Br}_x\text{Co(I)}]^-$ lead to the stepwise elimination of Br groups to give $[(\text{TPP})\text{Co(I)}]^-$ as a final product in solution. Results obtained by controlled-potential thin-layer spectroelectrochem. and rotating ring disk electrode voltammetry confirm this exptl. observation.

IT 131214-86-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with cobalt acetate)

RN 131214-86-3 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)



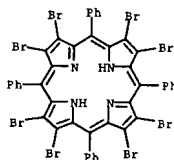
L6 ANSWER 127 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

L6 ANSWER 128 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1993:547430 CAPLUS
 DOCUMENT NUMBER: 119:147430
 TITLE: Structure of nonplanar octabromotetraphenylporphyrin and kinetics of rapid metalation reactions
 AUTHOR(S): Bhayappa, Puttaih; Nethaji, Munirathinam; Krishnan, Varadachari
 CORPORATE SOURCE: Dep. Inorg. Phys. Chem., Indian Inst. Sci., Bangalore, 560 012, India
 SOURCE: Chemistry Letters (1993), (5), 869-72
 CODEN: CHLTAG; ISSN: 0366-7022
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The crystal structure of 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenylporphyrin (H2L) show that it adopts a severe saddle-shaped distorted structure owing to the steric crowding of heavy Br substituents. Kinetic studies indicate the rate enhancement of H2L metalation reaction is primarily due to the nonplanarity of the ring while the electronic effect diminishes the affinity of the porphyrin towards metal ions.
 IT 150045-60-6, 2,3,7,8,12,13,17,18-Octabromo-5,10,15,20-tetraphenylporphyrin diethanolate dihydrate
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (crystal structure and kinetics of metalation of, by transition metal(II) cations)
 RN 150045-60-6 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-, compd. with ethanol (1:2), dihydrate (9CI) (CA INDEX NAME)

CM 1

CRN 131214-86-3
 CMF C44 H22 Br8 N4



CM 2

CRN 64-17-5
 CMF C2 H6 O

H₃C-CH₂-OH

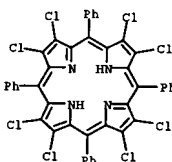
L6 ANSWER 129 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1993:191408 CAPLUS
 DOCUMENT NUMBER: 118:191408
 TITLE: Structure of meso-tetraaryl-β-octahalogenoporphyrins: a semi-empirical quantum-mechanical investigation
 AUTHOR(S): Brigaud, O.; Battioni, P.; Mansuy, D.
 CORPORATE SOURCE: Lab. Chim. Biochim. Pharmacol. Toxicol., Univ. Rene Descartes, Paris, 75270, Fr.
 SOURCE: New Journal of Chemistry (1992), 16(11), 1031-8
 CODEN: NJCHE5; ISSN: 0398-9836
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB AM1 calcs. were performed on 3 series of porphyrins, namely β-octahalogenoporphyrins, meso-tetraphenylporphyrins and meso-tetraaryl-β-octahalogenoporphyrins and on their zinc complexes. In the case of meso-tetraphenylporphyrins and β-octahalogenoporphyrins, a planar structure of the tetrapyrrole ring is the most stable one, as expected. On the contrary, the preferred conformation of meso-tetraaryl-β-octabromo(chloro)porphyrins and their zinc complexes corresponds to a saddle shape structure. For instance, the saddle conformation of 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenylporphyrin is more stable by 59 kJ/mol than the corresponding planar conformation. The best, energy wise, conformations are obtained by rotation of the pyrrole rings about the Cmeso-Cmeso lines and only to a much smaller extent about the pyrrole Cα-Cα lines. The stability of the conformations in which the meso carbons are no longer in the same plane (twist) decreases rapidly with the magnitude of this distortion. For saddle shape conformations, the Ph rings are no longer perpendicular to the porphyrin mean plane. The presence of bulky substituents on both β and meso carbon atoms is essential to obtain this type of structure. These results are in good agreement with recent x-ray studies on β-substituted meso-tetraarylporphyrins. The variation of the spacing and ordering of the frontier orbitals obtained in ruffled porphyrins is discussed in relation with exptl. data on metalloporphyrins π-radical cations.

IT 120644-25-9 131214-86-3 144811-83-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (AM1 MO calcs. of, conformation in relation to)

RN 120644-25-9 CAPLUS

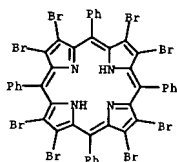
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-, (9CI) (CA INDEX NAME)



RN 131214-86-3 CAPLUS

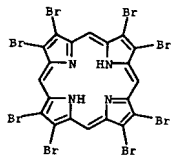
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-, (9CI) (CA INDEX NAME)

L6 ANSWER 129 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 144811-83-6 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo- (9CI) (CA INDEX NAME)



L6 ANSWER 130 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1993:6776 CAPLUS
 DOCUMENT NUMBER: 118:6776
 TITLE: Electronic effects of peripheral substituents in porphyrins: x-ray photoelectron spectroscopy and ab initio self-consistent field calculations
 AUTHOR(S): Gassman, Paul G.; Ghosh, Abhik; Almlof, Jan
 CORPORATE SOURCE: Dep. Chem., Univ. Minnesota, Minneapolis, MN, 55455, USA
 SOURCE: Journal of the American Chemical Society (1992), 114(25), 9990-10000
 CODEN: JACSAT; ISSN: 0002-7063
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The electronic effects of a wide variety of peripheral substituents in free base porphyrins have been evaluated using XPS and all-electron ab initio calcs. Both methods have identified the 1s energies of the central N atoms as excellent sensors of the electronic effects of peripheral substituents. Core level photoelectron spectra are reported for nine porphyrins, including unsubstituted porphyrin, octaethylporphyrin, and seven tetraphenylporphyrins. Substituents on the Ph groups in tetraphenylporphyrins modulate the electronic environment of the central region of the porphyrin nucleus in a significant manner. Thus, between tetraphenylporphyrin and tetrakis(pentafluorophenyl)porphyrin, the XPS nitrogen 1s ionization potentials shift by 0.9 eV. Ab initio SCF calcs. were carried out on substituted porphyrins, with multiple alkyl, aryl, fluoro, chloro, bromo, cyano, and nitro groups, using basis sets of double-ζ quality. Calcs. on selected porphyrins with larger, polarized basis sets suggest that both the absolute values of the orbital energies and the substituent effects are reasonably well converged at the double-ζ level of basis sets. Very large substituent effects (54.1 eV, relative to octamethylporphyrin) on the 1s energies of the central N atoms of the porphyrin nucleus are predicted for certain arrays of electron-withdrawing peripheral substituents. Valence orbital energies have also been computed, and the differences in the UV photoelectron spectra of porphyrin and octaalkylporphyrins are well reproduced by the calcs. Suitable arrays of strongly electron-withdrawing substituents result in large stabilizations of the porphyrin π orbitals, which should translate into enhanced stability of the porphyrins toward oxidative degradation. The molcs. studied by the ab initio calcs. range in size from porphyrin, C₂₀H₁₄N₄, to β-octafluoro-meso-tetrakis(pentafluorophenyl)porphyrin, C₄₄H₂F₂₀N₄. Use of the direct SCF formalism, in which integrals do not need to be stored, has made these large calcs. feasible. These calcs. demonstrate that at present ab initio calcs. can be performed routinely for molcs. containing 50-100 atoms.

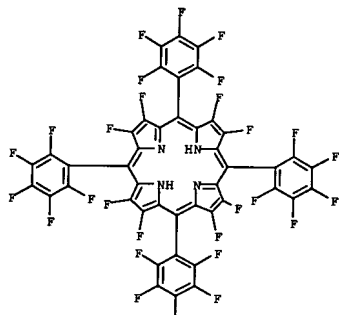
IT 121399-88-0 144811-81-4 144811-82-5
 144811-83-6 144811-86-9 144811-87-0
 144811-92-7

RL: RCT (Reactant); RACT (Reactant or reagent)
 (electronic effect of peripheral substituent in, MO calcn. of)

RN 121399-88-0 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

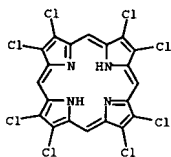
PAGE 1-A



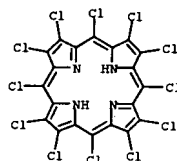
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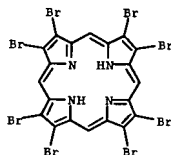
RN 144811-81-4 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro- (9CI) (CA INDEX NAME)



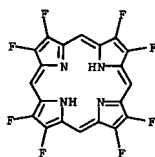
RN 144811-82-5 CAPLUS
CN 21H,23H-Porphine, 2,3,5,7,8,10,12,13,15,17,18,20-dodecachloro- (9CI) (CA INDEX NAME)



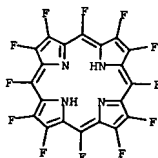
RN 144811-83-6 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo- (9CI) (CA INDEX NAME)



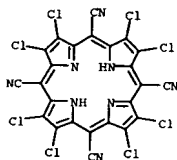
RN 144811-86-9 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro- (9CI) (CA INDEX NAME)



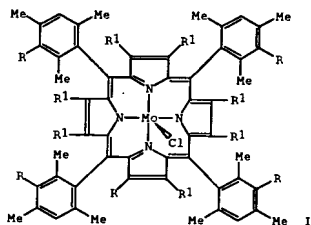
RN 144811-87-0 CAPLUS
CN 21H,23H-Porphine, 2,3,5,7,8,10,12,13,15,17,18,20-dodecafluoro- (9CI) (CA INDEX NAME)



RN 144811-92-7 CAPLUS
CN 21H,23H-Porphine-5,10,15,20-tetracarbonitrile, 2,3,7,8,12,13,17,18-octachloro- (9CI) (CA INDEX NAME)

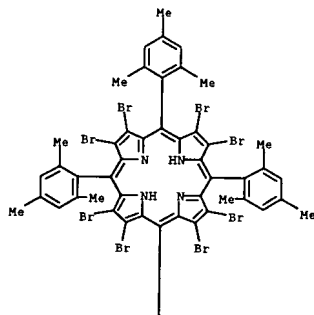


L6 ANSWER 131 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1992:633728 CAPLUS
DOCUMENT NUMBER: 117:233728
TITLE: Preparation and catalytic activities of molybdenum halogenated porphyrins in hydrogen peroxide olefin oxidations
AUTHOR(S): Hoffmann, Pascal; Meunier, Bernard
CORPORATE SOURCE: Lab. Chim. Coord., CNRS, Toulouse, 31077, Fr.
SOURCE: New Journal of Chemistry (1992), 16(5), 559-61
CODEN: NJCHE5; ISSN: 0398-9836
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 117:233728
GI

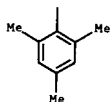


AB MoIII(Br8TMP)Cl (TMP = meso-tetramesitylporphyrinato) (I, R = H, R1 = Br) and MoIII(Cl12TMP)Cl (I, R = R1 = Cl) catalyze the epoxidn. of cyclooctene by 30% hydrogen peroxide in Et acetate at 70°.
IT 129006-48-0
RL: RCT (Reactant); RACT (Reactant or reagent) (metalation of, with molybdenum hexacarbonyl)
RN 129006-48-0 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

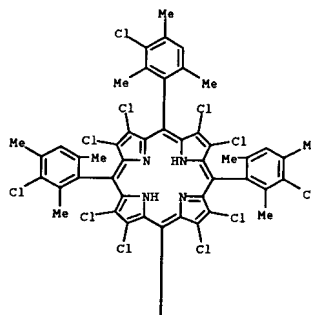
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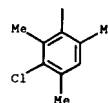
PAGE 2-A



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IT 141573-97-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and metalation of, with molybdenum hexacarbonyl)
 RN 141573-97-9 CAPLUS
 CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(3-chloro-2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 132 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1992:492626 CAPLUS
 DOCUMENT NUMBER: 117:92626
 TITLE: Metal coordination complex catalysts containing a halogenated ligand for hydrocarbon oxidation
 INVENTOR(S): Ellis, Paul E., Jr.; Lyons, James E.; Myers, Harry K., Jr.
 PATENT ASSIGNEE(S): Sun Refining and Marketing Co., USA
 SOURCE: Eur. Pat. Appl., 7 pp.
 CODEN: EPXKDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 11
 PATENT INFORMATION:

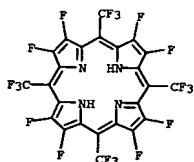
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 471561	A2	19920219	EP 1991-307493	19910814
EP 471561	A3	19920226		
R: BE, DE, FR, GB, IT, NL				
NO 9103150	A	19920217	NO 1991-3150	19910813
CA 2049177	AA	19920217	CA 1991-2049177	19910814
JP 05138037	A2	19930601	JP 1991-229785	19910816
US 5663328	A	19970902	US 1996-672202	19960627
PRIORITY APPL. INFO.:				
US 1990-568116 A 19900816				
US 1987-246 A2 19870102				
US 1987-66666 A2 19870626				
US 1989-425089 B2 19891023				
US 1994-303106 A3 19940907				

OTHER SOURCE(S): MARPAT 117:92626

AB The catalysts, useful for oxidation of alkanes, are perhalogenated porphyrin or perhalogenated phthalocyanine metal complexes (metal = Fe, Cr, Mn, Ru, and/or Cu), and are used to catalyze air or O₂ oxidation of aliphatic hydrocarbons. Thus, air oxidation of isobutane in C₆H₆ at 80° in presence of 0.013 mmol Fe(TPPF20Br8)Cl (TPP = tetraphenylporphyrin moiety) gave 89 mol tert-BuOH/100 mol liquid product and 3135 mol O₂ consumed/mol catalyst.

IT 142873-10-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with ferrous chloride)

RN 142873-10-7 CAPLUS
 CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(trifluoromethyl)- (9CI) (CA INDEX NAME)



L6 ANSWER 133 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN

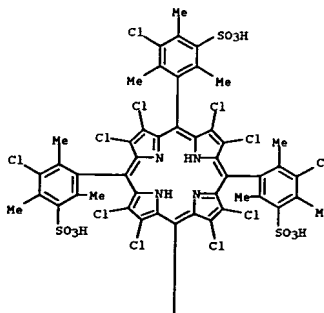
ACCESSION NUMBER: 1992:447538 CAPLUS
 DOCUMENT NUMBER: 117:47538
 TITLE: Olefin epoxidation and alkane hydroxylation catalyzed by robust sulfonated manganese and iron porphyrins supported on cationic ion-exchange resins
 AUTHOR(S): Campestrini, Sandro; Meunier, Bernard
 CORPORATE SOURCE: Lab. Chim. Coord., CNRS, Toulouse, 31077, Fr.
 SOURCE: Inorganic Chemistry (1992), 31(11), 1999-2006
 CODEN: INOCAJ; ISSN: 0020-1669
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 117:47538

AB Robust sulfonated manganese and iron porphyrins supported on poly(vinylpyridinium) polymers have been used as catalysts in olefin epoxidn. and alkane hydroxylation by iodosylbenzene. The metalloporphyrins are attached to protonated or methylated poly(vinylpyridine) polymers by the coordination of one pyridine unit, thus providing a proximal effect, and by addnl. interactions of the porphyrin sulfonate groups with the polymer pyridinium units. The best catalysts are the complexes containing halogen atoms at the pyrrole β-positions. In all these oxygenation reactions manganese porphyrins are better catalysts than the corresponding iron complexes. Comparative studies with another ion-exchange resin without a potential axial ligand show that the proximal effect is a key factor in metalloporphyrin-catalyzed reactions, not only for soluble complexes but also for supported catalysts.

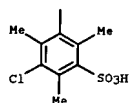
IT 142068-64-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and complexation with manganese)

RN 142068-64-2 CAPLUS
 CN Benzenesulfonic acid, 3,3',3'',3'''-(2,3,7,8,12,13,17,18-octachloro-21H, 23H-porphine-5,10,15,20-tetrayl)tetrakis(5-chloro-2,4,6-trimethyl-, tetrasodium salt (9CI) (CA INDEX NAME)

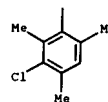
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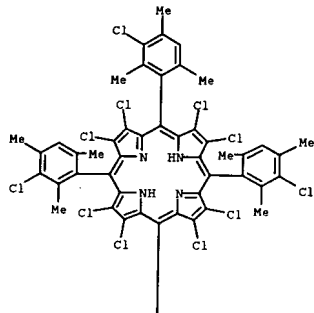
IT 141573-97-9

RL: RCT (Reactant); RACT (Reactant or reagent)
(sulfonation of)

RN 141573-97-9 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(3-chloro-2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

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L6 ANSWER 134 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1992:434399 CAPLUS

DOCUMENT NUMBER: 117:34399

TITLE: Preparation and catalytic activity of the manganese(III) dodecachlorotetramesitylporphyrin complex

AUTHOR(S): Hoffmann, Pascal; Robert, Anne; Meunier, Bernard

CORPORATE SOURCE: Lab. Chim. Coord., CNRS, Toulouse, 31077, Fr.

SOURCE: Comptes Rendus de l'Academie des Sciences, Serie II: Mecanique, Physique, Chimie, Sciences de la Terre et de l'Univers (1992), 314(1), 51-6

CODEN: CRAMED; ISSN: 0764-4450

DOCUMENT TYPE: Journal

LANGUAGE: French

AB Chloration with N-chlorosuccinimide of the zinc complex of tetramesitylporphyrin gives, after demetalation, the free porphyrin ligand meso-tetrakis(3-chloro-2,4,6-trimethylphenyl)-β-octachloroporphyrin, H₂C112TMP. The manganese and iron complexes of this new halogenated porphyrin were prepared. The catalytic activity of Mn(C112TMP)Cl was evaluated and compared with the activities of Mn(TMP)Cl and Mn(Br8TMP)Cl, when these catalysts are associated with potassium monopersulfate or magnesium monoperoxophthalate as oxygen donors. An abridged English version is included.

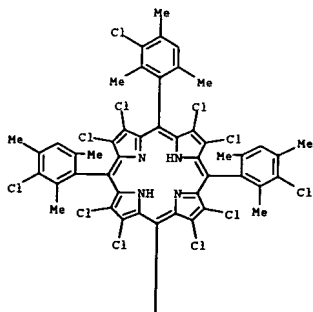
IT 141573-97-9p

RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(preparation and metalation of, in catalyst preparation)

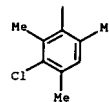
RN 141573-97-9 CAPLUS

CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(3-chloro-2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

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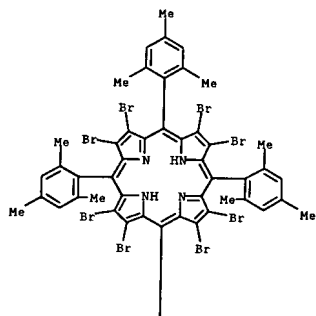


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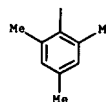
L6 ANSWER 135 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1992:426161 CAPLUS
 DOCUMENT NUMBER: 117:26161
 TITLE: Preparation and catalytic activities of the manganese and iron derivatives of Br8TMP and Cl12TMP, two robust porphyrin ligands obtained by halogenation of tetramesitylporphyrin
 AUTHOR(S): Hoffmann, P.; Robert, A.; Meunier, B.
 CORPORATE SOURCE: Lab. Chim. Coord., CNRS, Toulouse, 31077, Fr.
 SOURCE: Bulletin de la Societe Chimique de France (1992), 129(1), 85-97
 CODEN: BSCFAS; ISSN: 0037-8968
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The ionic halogenation of tetramesitylporphyrin by N-bromosuccinimide or N-chlorosuccinimide gives, as main product, meso-tetramesityl- β -octabromoporphyrin (H2Br8TMP) and meso-tetrakis(3-chloro-2,4,6-trimethylphenyl)- β -octachloroporphyrin (H2Cl12TMP), resp. Both Mn and Fe derivs. of these two porphyrins are efficient catalysts for olefin epoxidn. and alkane hydroxylation. The kinetic isotope effects of hydroxylation reactions were determined using different porphyrin catalysts and various O atom donors. The kH/kD values ranged from 2 ± 0.8 to 9 ± 3 and were more dependent on the nature of the central metal and the oxidant than on the structure of the porphyrin ligand itself. PhIO is the only O atom donor in association with Fe porphyrins able to give high kinetic isotope effects (7.7 to 9.0) close to the primary isotope effects reported for cytochrome P 450 itself.
 IT 129006-48-0P 141573-97-9P
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and complexation of)
 RN 129006-48-0 CAPLUS
 CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

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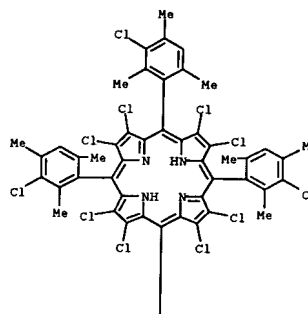
L6 ANSWER 135 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

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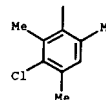


RN 141573-97-9 CAPLUS
 CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(3-chloro-2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

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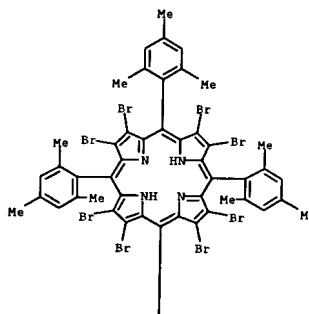
PAGE 2-A



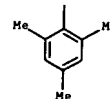
L6 ANSWER 136 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1992:247254 CAPLUS
 DOCUMENT NUMBER: 116:247254
 TITLE: β -Halogenated-pyrrole porphyrins. Molecular structures of 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetramesitylporphyrin, nickel(II) 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetramesitylporphyrin, and nickel(II) 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(pentafluorophenyl)porphyrin
 AUTHOR(S): Mandon, D.; Ochenbein, P.; Fischer, J.; Weiss, R.; Jayaraj, K.; Austin, R. N.; Gold, A.; White, P. S.; Brigaud, O.; et al.
 CORPORATE SOURCE: Inst. LeBel, Univ. Louis Pasteur, Strasbourg, F-67070, Fr.
 SOURCE: Inorganic Chemistry (1992), 31(11), 2044-9
 CODEN: INOCAJ; ISSN: 0020-1669
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The x-ray structures of the β -substituted-pyrrole tetraarylporphyrin 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetramesitylporphyrin (H2TMOBP), Ni(TMOBP), and Ni(TFPPOBP-1/2CH2Cl2) (H2TFPPOBP-1/2CH2Cl2) are reported. The synthesis of H2TFPPOBP-1/2CH2Cl2 (H2TFPPOBP-1/2CH2Cl2) is described. All these mols. are nonplanar, displaying saddle-shaped conformations. The saddle distortions minimize the intramol. steric interactions between the Br substituents and the ortho (ortho') C atoms or ortho (ortho') substituents of the Ph rings, and consequently, the corresponding contact distances have similar values in all compds. Because of the distortion of the porphyrin cores, the cavity defined by the ortho (ortho') substituents gives slightly less steric protection than in the nonbrominated nearly planar ortho- and ortho'-substituted tetraarylporphyrin complexes. Crystallog. data: H2TMOBP: tetragonal, space group P4hvin.421c, Z = 2, R = 0.054, Rw = 0.069; Ni(TMOBP): tetragonal, space group P4hvin.421c, Z = 2, R = 0.049, Rw = 0.057; Ni(TFPPOBP-1/2CH2Cl2): monoclinic, space group C2/c, Z = 8, R = 0.047, Rw = 0.064.
 IT 129006-48-0
 RL: RCT (Reactant); RACT (Reactant or reagent) (crystal structure and reaction of, with nickel acetate)
 RN 129006-48-0 CAPLUS
 CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 136 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

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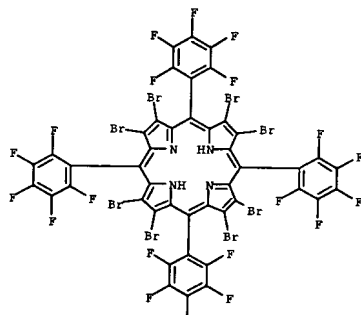


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IT 139944-26-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and reaction of, with nickel acetate)
 RN 139944-26-6 CAPLUS
 CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

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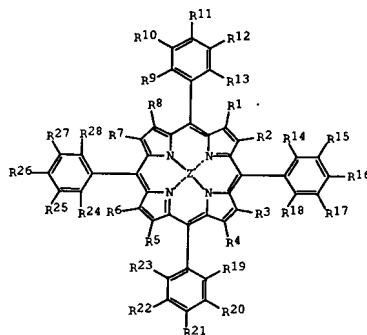
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L6 ANSWER 137 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1992:213987 CAPLUS
 DOCUMENT NUMBER: 116:213987
 TITLE: Oxidation of olefins with oxygen catalyzed by halogenated porphyrin complexes
 INVENTOR(S): Tsuchiya, Shinji; Kawai, Motomasu
 PATENT ASSIGNEE(S): Mitsui Toatsu Chemicals, Inc., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
 CODEN: JKKXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 03246238	A2	19911101	JP 1990-42342	19900226
JP 2790885	B2	19980827	JP 1990-42342	19900226

PRIORITY APPLN. INFO.: MARPAT 116:213987
 OTHER SOURCE(S): GI

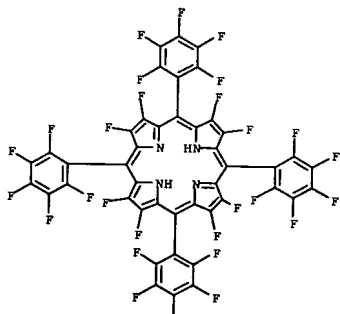


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AB Olefinic compds. are oxidized with O to O-containing compds. in the presence of I [R1 - R28 = Cl-4 alkyl, trihalomethyl, H, halo; Z of R1 - R28 is halo; Z consisting of a cation of n valence (Mn+) from Groups IA to VIA, IB to VIIIB, and VIII elements and an anion (X-) from O, F-, Cl-, Br-, I-, O-, OH-, MeO-, EtO-, PrO-, i-PrO-, tert-C₄H₉O-, PhO-, AcO-, CN-, CSN-, and ClO₄- in the form of 2M+, H₂M+, M₂+, M₃X-, M₄X-2, OM₄+, or OM₅X-; n = 1-5]. The reaction may be carried out in the presence of a base (for example, alc. and typically MeOH) and the process is applicable to propylene, 1-butene, 2-butene, butadiene, isoprene, cyclopentene,

L6 ANSWER 137 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
 cycloheptene, cyclooctene, 1,4-cyclooctadiene, styrene, α-methylstyrene, β-methylstyrene, stilbene, allyl chloride, allyl bromide, allyl alc., oleic acid, and oleic acid esters. Thus, stirring 7 mmol cyclooctene with air at 25° in the presence of 1 μmol 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)porphyrinatoiron (III) chloride gave 0.08 mmol 1,2-epoxycyclooctane vs. 0.01 mmol in the presence of tetrakis(2,4,6-trimethylphenyl)porphyrinatoiron (III).
 IT 121399-88-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reaction of, with ferric chloride)
 RN 121399-88-0 CAPLUS
 CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

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L6 ANSWER 138 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1992:106069 CAPLUS
 DOCUMENT NUMBER: 116:106069
 TITLE: Porphine complexes as oxidation catalysts for olefins
 INVENTOR(S): Tsuchiya, Shinji; Senoo, Manabu; Kawai, Motomasu
 PATENT ASSIGNEE(S): Mitsui Toatsu Chemicals, Inc., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
 CODEN: JKKXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

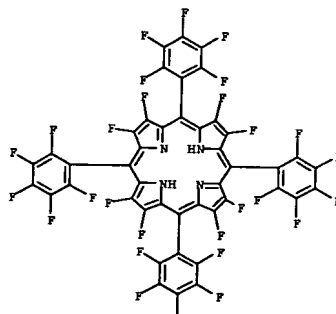
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 03232534	A2	19911016	JP 1990-27219	19900208
JP 03232534	A2	19911016	JP 1990-27219	19900208

PRIORITY APPLN. INFO.: CASREACT 116:106069; MARPAT 116:106069
 OTHER SOURCE(S): AB Epoxides and oxygen-containing compound were prepared by oxidation of olefins with

oxygen in the presence of porphine complexes and alcs or amines. Thus, air oxidation of 3 mmol cyclohexene in CH₂Cl₂ in the presence of 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)porphyrinatoiron(III) chloride and MeOH at 25° for 2 h gave 0.15 mmol oxidation products 1,2-epoxycyclohexene, cyclohex-2-en-1-ol, and cyclohex-2-en-1-one in a ratio of 22:30:48.

IT 121399-88-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reaction of, with ferric chloride)
 RN 121399-88-0 CAPLUS
 CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

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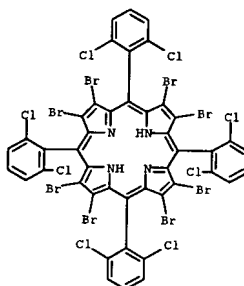
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L6 ANSWER 139 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1991:523796 CAPLUS
 DOCUMENT NUMBER: 115:123796
 TITLE: Silver halide color photographic material containing porphyrin for black spot prevention
 INVENTOR(S): Kawasaki, Mikio
 PATENT ASSIGNEE(S): Konica Co., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.
 CODEN: JKOXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

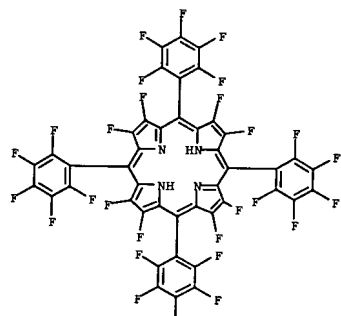
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JF 03041441	A2	19910221	JP 1989-177732	19890707
PRIORITY APPL. INFO.:			JP 1989-177732	19890707
OTHER SOURCE(S):		MARPAT 115:123796		

AB A photog. material contains ≥ 1 porphyrin derivative in the ≥ 1 hydrophilic layer on the support. It prevents the image layer from subjecting to generation of microspot defects, and is suitably applied to x-ray film for medical diagnosis. $\alpha, \beta, \gamma, \delta$ -Tetraphenylporphyrin was added into the Ag(Br,I) emulsion for a black-and-white film for x-ray diagnosis.
 IT 107035-95-0 121399-88-0 135762-91-3
 RL: DEV (Device component use); USES (Uses)
 (x-ray photog. film containing, for black spot prevention)
 RN 107035-95-0 CAPLUS
 CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,6-dichlorophenyl)- (9CI) (CA INDEX NAME)



RN 121399-88-0 CAPLUS
 CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

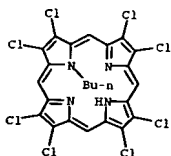
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RN 135762-91-3 CAPLUS
 CN 21H, 23H-Porphine, 21-butyl-2,3,7,8,12,13,17,18-octachloro- (9CI) (CA INDEX NAME)

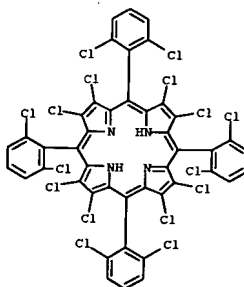


ACCESSION NUMBER: 1991:514223 CAPLUS
 DOCUMENT NUMBER: 115:114223
 TITLE: Metal-assisted reactions. Part 22. Synthesis of perhalogenated porphyrins and their use as oxidation catalysts
 AUTHOR(S): Gonsalves, Antonio M. D Rocha; Johnstone, Robert A. W.; Pereira, Mariette M.; Shaw, Jacqueline; Sobral, Abilio J. F. do N.
 CORPORATE SOURCE: Dep. Quim., Univ. Coimbra, Coimbra, 3000, Port.
 SOURCE: Tetrahedron Letters (1991), 32(10), 1355-8
 CODEN: TELEAY; ISSN: 0040-4039
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB meso-Tetraarylporphyrins have been perchlorinated and perbrominated at peripheral (β)-positions of the pyrrole rings by high-yielding procedures. These halogenated porphyrins show enhanced catalytic activity towards oxidation of alkanes and alkenes but are not stable when H2O2 is used as the O donor. The reason for this instability appears to lie in excessive homolytic dissociation of H2O2 with consequent rapid attack at the porphyrin β-position.

IT 134833-67-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and complexation of, with manganese)

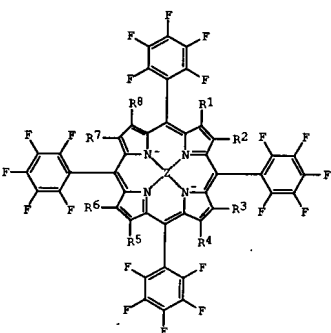
RN 134833-67-3 CAPLUS
 CN 21H, 23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetrakis(2,6-dichlorophenyl)- (9CI) (CA INDEX NAME)



L6 ANSWER 141 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1991:479933 CAPLUS
 DOCUMENT NUMBER: 115:79933
 TITLE: Fluorine-substituted porphyrin complex for oxidation catalyst of organic compound
 INVENTOR(S): Tsuchida, Shinji; Senoo, Manabu; Kawai, Motomasa
 PATENT ASSIGNEE(S): Mitsui Toatsu Chemicals, Inc., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
 CODEN: JKKXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

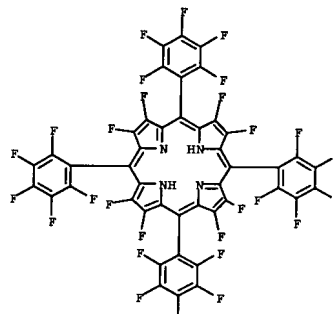
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02250883	A2	19901008	JP 1989-241912	19890920
JP 2845982	B2	19990113		

PRIORITY APPLN. INFO.: JP 1988-310051 A1 19881209
 OTHER SOURCE(S): MARPAT 115:79933
 GI



L6 ANSWER 141 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
 RN 121399-88-0 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-tetrakis(pentafluorophenyl)-(9CI) (CA INDEX NAME)

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AB The complex is I [R1-8 = H, F (≥1); Z = Group IA-VIA, cation (M⁺-5+), of Group IV-VIIB, VIII, and anion (X⁻) O, F⁻, Cl⁻, Br⁻, I⁻, O⁻, OH⁻, MeO⁻, EtO⁻, PrO⁻, Me2CO⁻, tert-BuO⁻, PhO⁻, AcO⁻, CN⁻, SCN⁻, and/or ClO4⁻; possible form 2M⁺, H⁺M⁺, M2⁺, M3⁺X⁻, M4⁺X⁻2, O:M4⁺, O:M5⁺X⁻]. An organic compound is oxidized by peroxides with the complex as a catalyst.
 IT 121399-88-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reaction of)

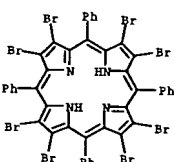
L6 ANSWER 142 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1991:54757 CAPLUS
 DOCUMENT NUMBER: 114:54757
 TITLE: Octabromotetraphenylporphyrin and its metal derivatives: Electronic structure and electrochemical properties
 AUTHOR(S): Bhayappa, P.; Krishnan, V.
 CORPORATE SOURCE: Dep. Inorg. Phys. Chem., Indian Inst. Sci., Bangalore, 560 012, India
 SOURCE: Inorganic Chemistry (1991), 30(2), 239-45
 CODEN: INOCAJ; ISSN: 0020-1669
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Free-base octabromotetraphenylporphyrin (H2OBP) was prepared by bromination of Cu(TPP) (H2TPP = meso-tetraphenylporphyrin). M(OBP) (M = VO2⁺, Co, Ni, Cu, Zn, Pd, Ag, Pt) exhibit interesting electronic spectral features and electrochem. redox properties. The electron-withdrawing Br substituents at the pyrrole C atoms in H2OBP and M(OBP) produce remarkable red shifts in the Soret (50 nm) and visible bands (100 nm) of the porphyrin. The low magnitude of protonation consts. (pK3 = 2.6 and pK4 = 1.75) and the large red-shifted Soret and visible absorption bands make the octabromoporphyrin unique. The effect of electroneg. Br substituents at the peripheral positions of the porphyrin was quant. analyzed by using the 4-orbital approach of M. J. Gouterman (1959). A comparison of MO parameters of M(OBP) with those of M(TPP) and M(Por) (H2Por = porphine) provides an explanation for the unusual spectral features. The Cl matrix element of M(OBP) is the lowest among the known substituted porphyrins, indicating delocalization of ring charge caused by the increase in conjugation of p orbitals of the Br onto the ring orbitals. The electron-transfer reactivities of the porphyrins are altered by the peripheral Br substituents, producing large anodic shifts in the ring and metal-centered redox potentials. The increase in anodic shift in the reduction potential

of M(OBP) relative to M(TPP) is large (550 mV) compared to the shift in the oxidation potential (300 mV). These results were interpreted in terms of the resonance and inductive interactions of the Br substituents.
 IT 131214-86-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and cyclic voltammetry and visible spectra and protonation

of) 131214-86-3 CAPLUS
 RN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetraphenyl-
 CN (9CI) (CA INDEX NAME)



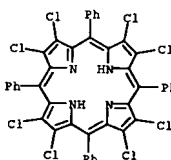
L6 ANSWER 143 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1990:564403 CAPLUS
 DOCUMENT NUMBER: 113:164403
 TITLE: Highly chlorinated and perchlorinated meso-tetraphenylporphyrins
 AUTHOR(S): Wijesekera, Tilak; Matsumoto, Akiteru; Dolphin, David; Lexa, Doris
 CORPORATE SOURCE: Dep. Chem., Univ. British Columbia, Vancouver, BC, V6T 1Y6, Can.
 SOURCE: Angewandte Chemie (1990), 102(9), 1073-4
 CODEN: ANCEAD; ISSN: 0044-8249
 DOCUMENT TYPE: Journal
 LANGUAGE: German

AB FeCl3 (H2L = meso-tetra(2,6-dichlorophenyl)porphyrin, tetra(perchlorophenyl)porphyrin) were chlorinated by Cl2 gas in the presence of FeCl3 in o-C6H4Cl2 to give FeCl3 (H2L1 = meso-tetra(2,6-dichlorophenyl)octachloroporphyrin, tetra(perchlorophenyl)octachloroporphyrin). Chlorination of Fe(TPP)Cl (H2TPP = tetraphenylporphyrin) by Cl/FeCl3 led to decomposition of the macrocycle. Fe(TPP)Cl and H2TPP were

only partially chlorinated by N-chlorosuccinimide (NCS). Ni(TPP) reacted with I in o-C6H4Cl2 to give NiI2 (H2L2 = octachloroporphyrin). Attempted chlorination of M(TPP) (M = Cu, Zn) led to ring opening. The effect of chlorination of the porphyrin coordinated to Fe was studied on the oxidation and reduction potentials in the presence of Cl⁻ and Ag⁺.
 IT 120644-25-9P

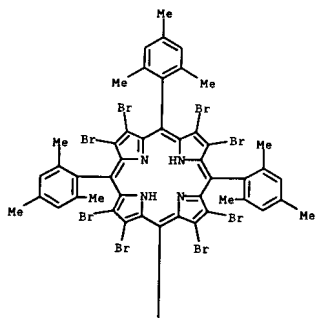
RL: FORM (Formation, nonpreparative); PREP (Preparation)
 (formation of, in demetallation of nickel complex)

RN 120644-25-9 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl-
 (9CI) (CA INDEX NAME)



L6 ANSWER 144 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1990:514910 CAPLUS
 DOCUMENT NUMBER: 113:114910
 TITLE: Highly selective bromination of tetramesitylporphyrin:
 an easy access to robust metalloporphyrins, M-Br8TMP
 and M-Br8TMPs. Examples of application in catalytic
 oxygenation and oxidation reactions
 Hoffmann, Pascal; Labat, Gilles; Robert, Anne;
 Meunier, Bernard
 CORPORATE SOURCE: Lab. Chim. Coord., CNRS, Toulouse, 31077, Fr.
 SOURCE: Tetrahedron Letters (1990), 31(14), 1991-4
 CODEN: TETLEA; ISSN: 0040-4039
 DOCUMENT TYPE: Journal
 LANGUAGE: English

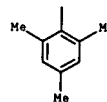
AB The N-bromosuccinimide bromination of the zinc derivative of
 meso-tetramesitylporphyrin, [Zn(TMP)], in MeOH under reflux in air, gives
 meso-tetramesityl- β -octabromoporphyrinatolactone [Zn(Br8TMP)], in high
 yield (60-75%). Furthermore, the sulfonation by oleum of the metal-free
 ligand Br8TMPH2 gives meso-tetrakis(3,5-disulfonatomesityl)- β -
 octabromoporphyrin, Br8TMPSH2 (70-75%). These manganese and iron derivs.,
 Mn(Br8TMP)Cl, Fe(Br8TMP)Cl, Mn(Br8TMP)S, and Fe(Br8TMP)S, are efficient
 catalysts in oxygen atom or electron transfer reactions.
 IT 129006-48-0P 129006-49-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and metalation of)
 RN 129006-48-0 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,4,6-
 trimethylphenyl)- (9CI) (CA INDEX NAME)



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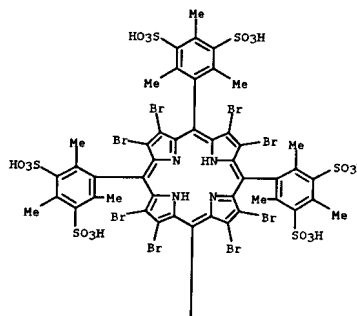
L6 ANSWER 144 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

PAGE 2-A

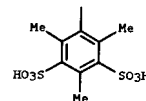


RN 129006-49-1 CAPLUS
 CN 1,3-Benzenedisulfonic acid, 5,5',5'',5'''-(2,3,7,8,12,13,17,18-octabromo-
 21H,23H-porphine-5,10,15,20-tetrayl)tetrakis(2,4,6-trimethyl- (9CI) (CA
 INDEX NAME)

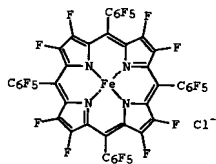
PAGE 1-A



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L6 ANSWER 145 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1989:457150 CAPLUS
 DOCUMENT NUMBER: 111:57150
 TITLE: Novel synthetic method of phenol from benzene
 catalyzed by perfluorinated hemin
 Tsuchiya, Shinji; Seno, Manabu
 CORPORATE SOURCE: Inst. Ind. Sci., Univ. Tokyo, Tokyo, 106, Japan
 SOURCE: Chemistry Letters (1989), (2), 263-6
 CODEN: CHLTAG; ISSN: 0366-7022
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 111:57150
 GI

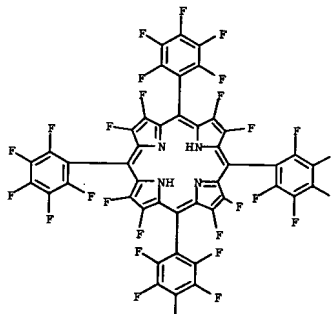


AB New perfluorinated hemin I catalyzes the hydroxylation of C6H6 by H2O2 at
 room temperature and 1 atm pressure. The turnover for PhOH produced in 2 h
 13 55. I also catalyzes the epoxidn. of cyclooctene by H2O2.

IT 121399-88-0
 RL: PROC (Process)
 (UV absorption of)
 RN 121399-88-0 CAPLUS
 CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octafluoro-5,10,15,20-
 tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 145 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

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F

L6 ANSWER 146 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1989:407144 CAPLUS
DOCUMENT NUMBER: 111:7144

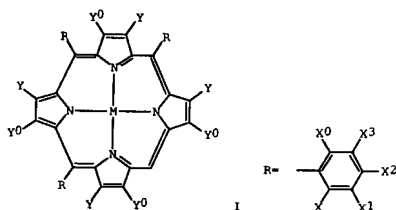
TITLE: Metalated tetraphenyl porphyrins, their nonmetalated precursors, and their use in the oxidation of lignin, alkanes, and alkenes
INVENTOR(S): Dolphin, David H.; Nakano, Taku; Kirk, Thomas Kent; Malone, Theodore E.; Farrell, Roberta L.; Wijesekera, Tilak Panini

PATENT ASSIGNEE(S): Can.
SOURCE: PCT Int. Appl., 46 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 8807988	A1	19881020	WO 1988-US1240	19880415
W1: AU, DK, FI, JP, KR, NO, SU				
RF: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
AU 8817075	B2	19881104	AU 1988-17075	19880415
AU 617670	A	19911205		
US 4892941	A	19900109	US 1988-181859	19880415
EP 363379	A1	19900418	EP 1988-904116	19880415
EP 363379	B1	19950614		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
JP 02503086	T2	19900927	JP 1988-503781	19880415
CA 1308096	A1	19920929	CA 1988-564424	19880418
NO 8805571	A	19881216	NO 1988-5571	19881215
DK 8807020	A	19881216	DK 1988-7020	19881216
KR 9702638	B1	19970307	KR 1988-71690	19881217
FI 92402	B	19940729	FI 1989-4898	19891016
FI 92402	C	19941110		
US 5077394	A	19911231	US 1989-455663	19891221
PRIORITY APPLN. INFO.:			US 1987-39566	A 19870417
			US 1988-181859	A3 19880415
			WO 1988-US1240	A 19880415

OTHER SOURCE(S): MARPAT 111:7144
GI

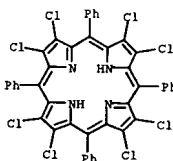


L6 ANSWER 146 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

AB Metalated porphyrins I [M = oxidation-sustaining transition metal, optionally with axial ligand; X, X0 = H, non-H2O-solubilizing electroneg. group; X1-X3 = H, electroneg. group; Y, Y0 = H, F, Cl; Y and/or Y0 = H when none of X1-X3 is H2O-soluble; 1-2 of X1-X3 is H2O-soluble and 2 of X's in non-H2O-soluble electroneg. group when Y = Y0 = H; 2 of X1-X3 is H2O-soluble] and their salt forms are prepared for use as oxidation catalysts, especially for oxidation-degradation of lignin in wood or pulp, hydroxylation of (cyclo)alkanes, and epoxidn. of (cyclo)alkenes. Chlorination of chloro[meso-tetra-(2,6-dichlorophenyl)porphyrinato]iron(III) using FeCl3 and Cl at 140° gave 88% of the β-octachloro derivative, which underwent demetalation-sulfonation by fuming H2SO4 at 165° and remetalation by FeCl2.4H2O in DMF to give I (M = Fe with axial Cl ligand, X = X0 = Cl, X1 = X2 = H, X3 = SO3H, Y = Y0 = Cl) (II). Oxidation of 2 g northern softwood kraft by 0.5% (w/v) Me3COOH in buffer at pH 5 and 60° yielded a kappa value of 9.5 in the presence of 90 mg II, vs. 17.6 without II.

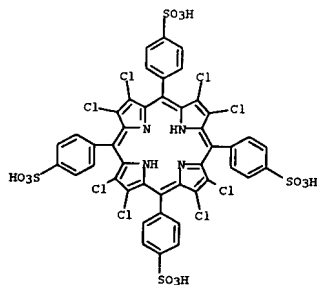
IT 120644-25-9P 120644-26-0P 120644-27-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and metalation of)

RN 120644-25-9 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octachloro-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)

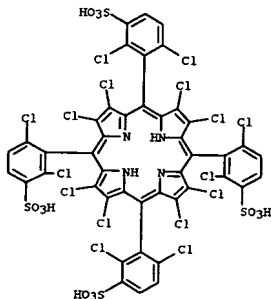


RN 120644-26-0 CAPLUS
CN Benzenesulfonic acid, 4,4',4'',4'''-(2,3,7,8,12,13,17,18-octachloro-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis- (9CI) (CA INDEX NAME)

L6 ANSWER 146 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 120644-27-1 CAPLUS
CN Benzenesulfonic acid, 3,3',3'',3'''-(2,3,7,8,12,13,17,18-octachloro-21H,23H-porphine-5,10,15,20-tetrayl)tetrakis(2,4-dichloro- (9CI) (CA INDEX NAME)



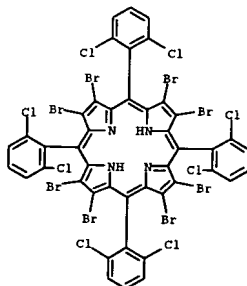
L6 ANSWER 147 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1989:107073 CAPLUS
DOCUMENT NUMBER: 110:107073

TITLE: Perhalogenated tetraphenylhemins: stable catalysts of high turnover catalytic hydroxylations [Erratum to document cited in CA106(18):148310d]
AUTHOR(S): Traylor, Teddy G.; Tsuchiya, Shinji
CORPORATE SOURCE: Dep. Chem., Univ. California, La Jolla, CA, 92093, USA
SOURCE: Inorganic Chemistry (1988), 27(24), 4520
CODEN: INOCAJ; ISSN: 0020-1669

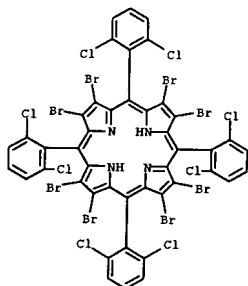
DOCUMENT TYPE: Journal
LANGUAGE: English
AB An error in Table I has been corrected. The error was not reflected in the abstract or the index entries.

IT 107035-95-0P
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of (Erratum))

RN 107035-95-0 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,6-dichlorophenyl)- (9CI) (CA INDEX NAME)



L6 ANSWER 148 OF 148 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1987:148310 CAPLUS
DOCUMENT NUMBER: 106:148310
TITLE: Perhalogenated tetraphenylhemins: stable catalysts of
high turnover catalytic hydroxylations
AUTHOR(S): Traylor, Teddy G.; Tsuchiya, Shinji
CORPORATE SOURCE: Dep. Chem., Univ. California, La Jolla, CA, 92093, USA
SOURCE: Inorganic Chemistry (1987), 26(8), 1338-9
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Bromination of tetrakis(2,6-dichlorophenyl)porphyrinatozinc affords the
2,3,7,8,12,13,17,18-octabromo compound (H2L) which is converted into FeLCl.
This hemin catalyzes high turnover, rapid hydroxylation of alkanes without
catalyst destruction.
IT 107035-95-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 107035-95-0 CAPLUS
CN 21H,23H-Porphine, 2,3,7,8,12,13,17,18-octabromo-5,10,15,20-tetrakis(2,6-
dichlorophenyl)- (9CI) (CA INDEX NAME)



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COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

733.37

909.57

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

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-108.04

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